=> d ibib abs hitstr 1

L29 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:591191 HCAPLUS
DOCUMENT NUMBER: 136:2011
TITLE: Inhibition of major groove DNA binding bZIP proteins by positive patch **polyamides**
AUTHOR(S): Bremer, R. E.; Wurtz, N. R.; Szewczyk, J. W.; Dervan, P. B.
CORPORATE SOURCE: Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, 91125, USA
SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(8), 2093-2103
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cell permeable synthetic ligands that bind to predetd. DNA sequences offer a chem. approach to gene regulation, provided inhibition of a broad range of DNA transcription factors can be achieved. DNA minor groove binding **polyamides** contg. aminoalkyl substituents at the N-1 of a single pyrrole residue display inhibitory effects for a bZIP protein which binds exclusively in the DNA major groove. For major groove protein inhibition, specific protein-DNA contacts along the **phosphate backbone** were targeted with the pos. charged dimethylamino substituent on the backbone of a minor groove binding **polyamide** hairpin. Remarkably, these **polyamides** bind DNA with enhanced affinity and uncompromised specificity when compared to **polyamides** with the aminoalkyl moiety at the C-terminus. By adding bZIP transcription factors to the class of protein-DNA complexes that can be disrupted by minor groove binding ligands, these results may increase the functional utility of **polyamides** as regulators of gene expression.

IT **180530-17-0 180530-18-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)

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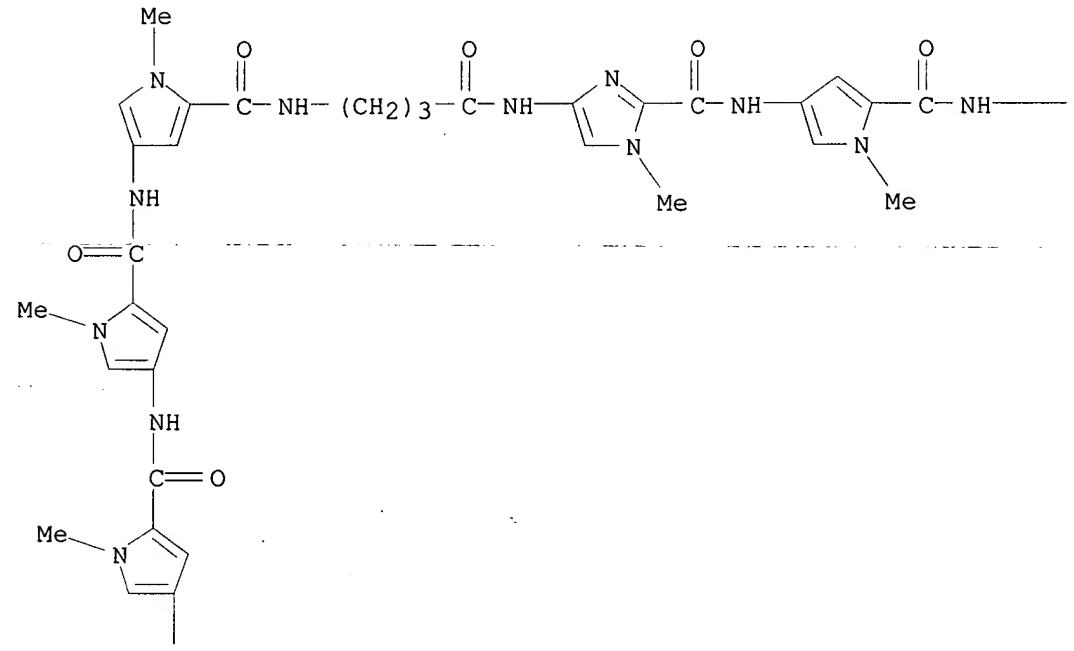

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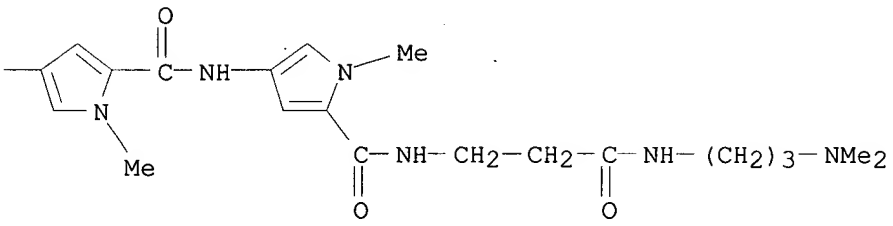

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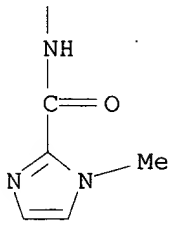

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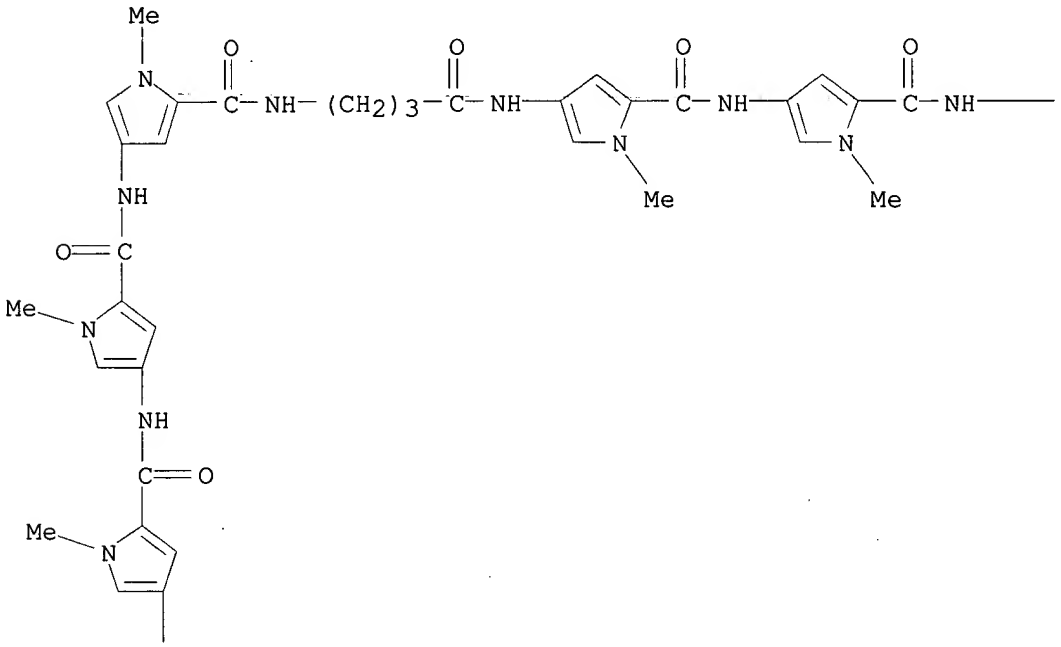

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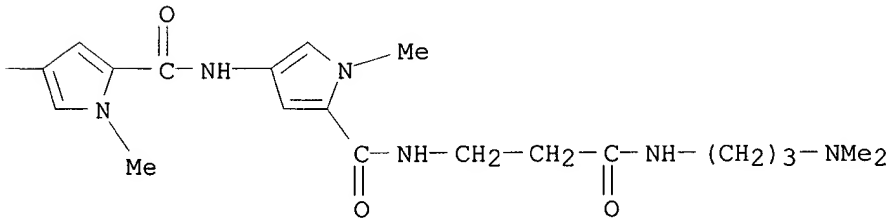

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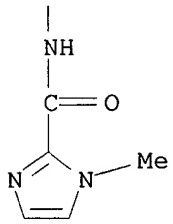

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374694-30-1P 374694-32-3P 374694-35-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)

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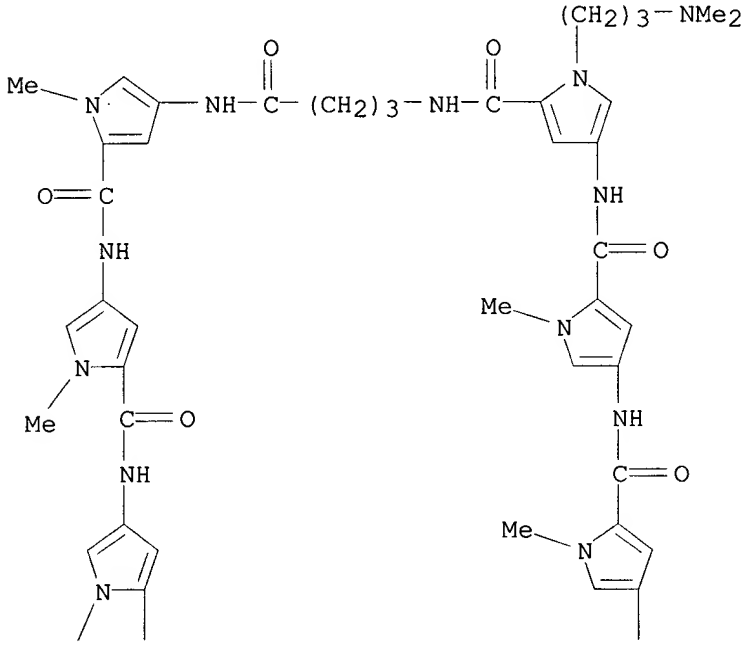

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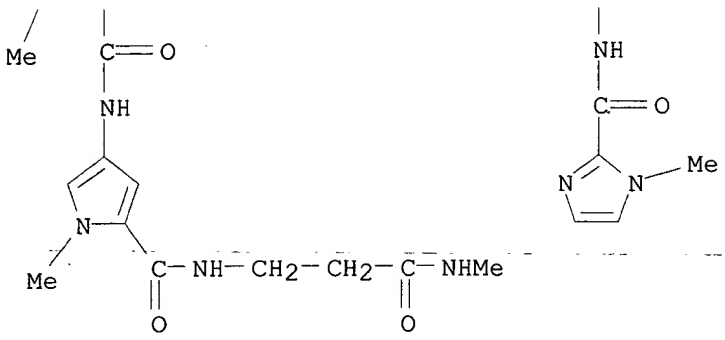

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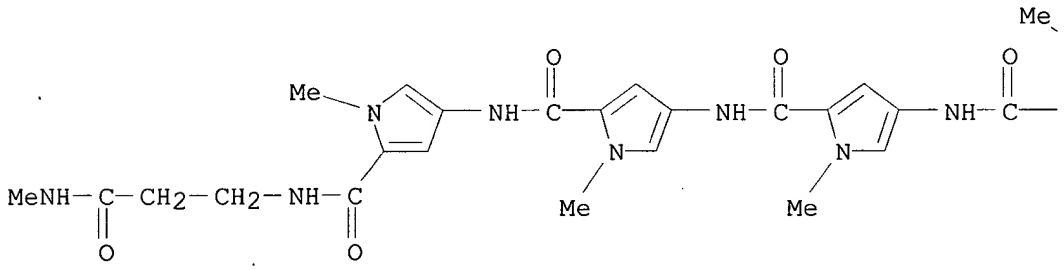

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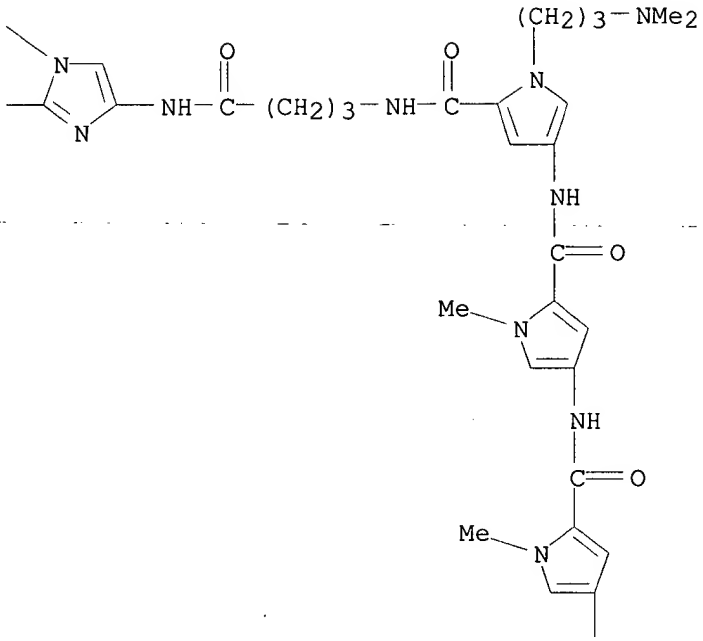

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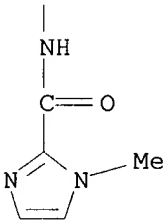

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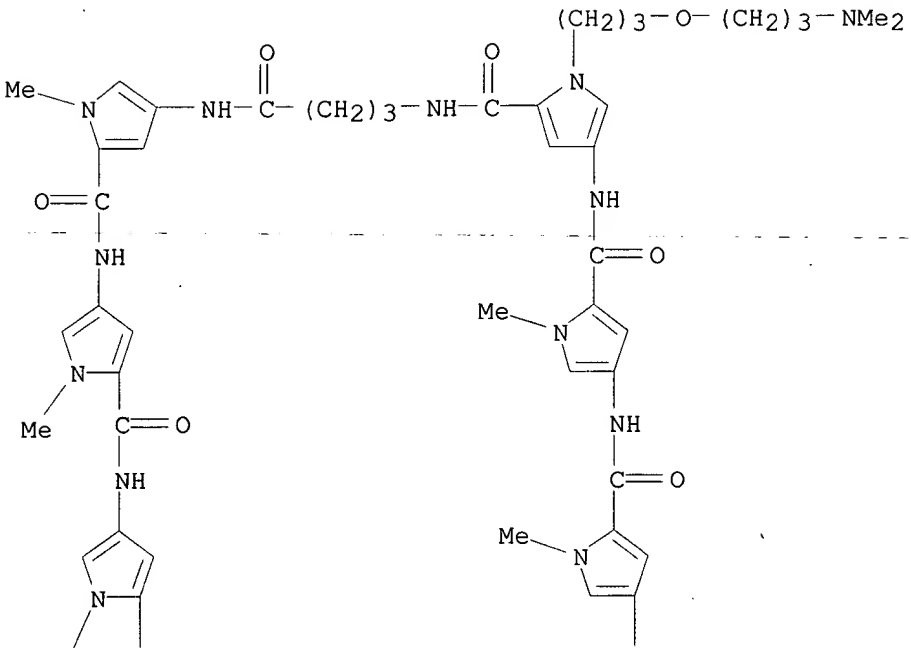

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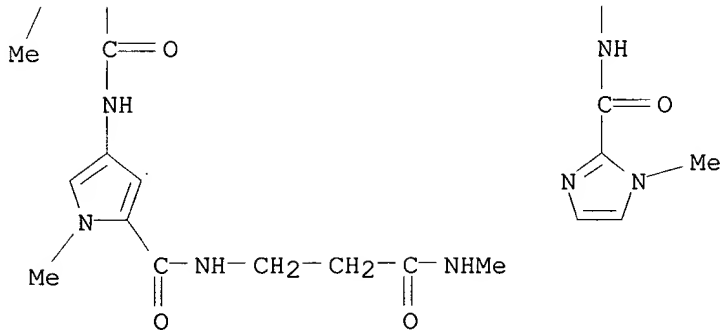

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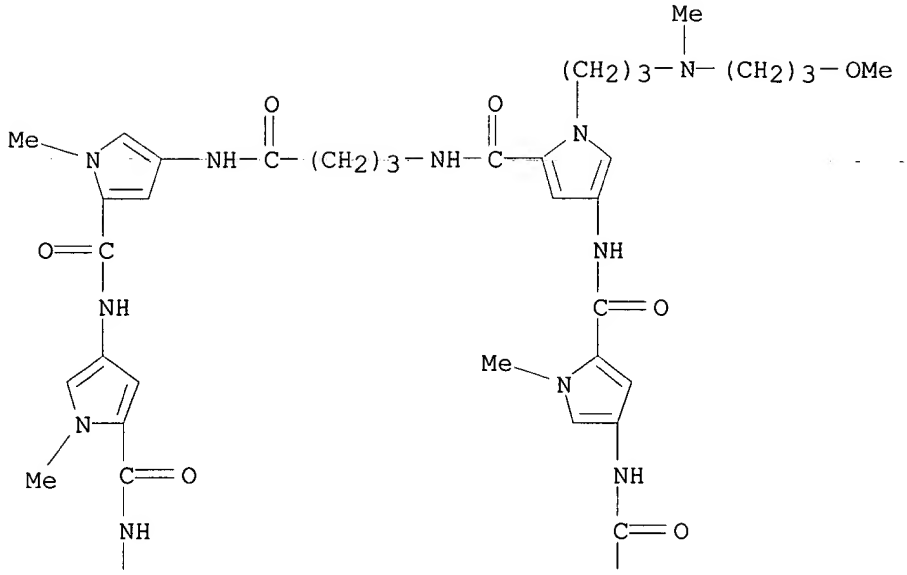

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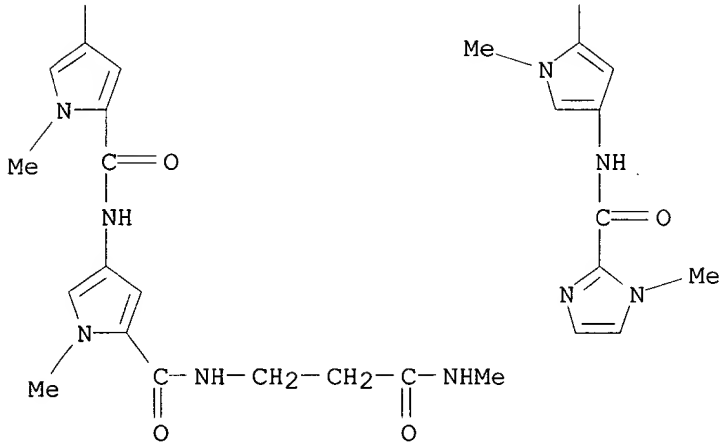

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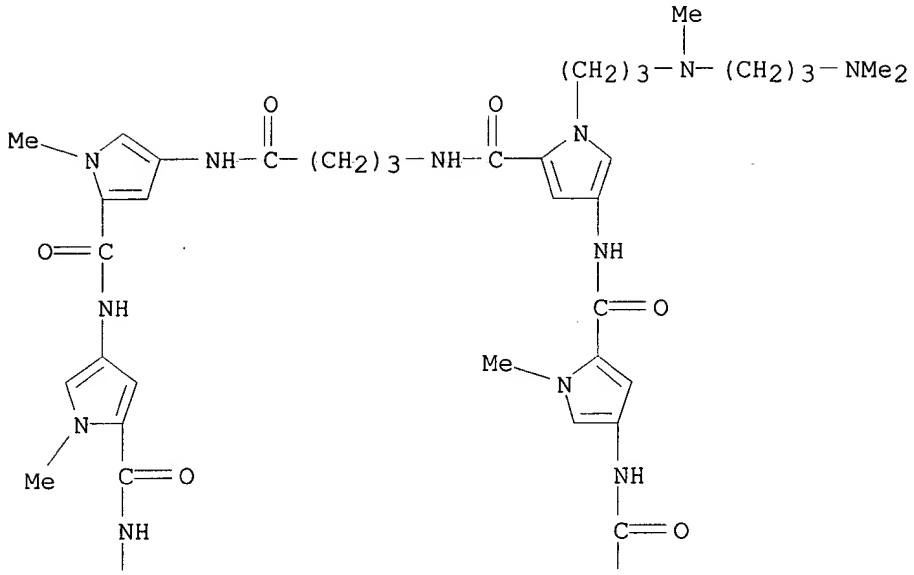

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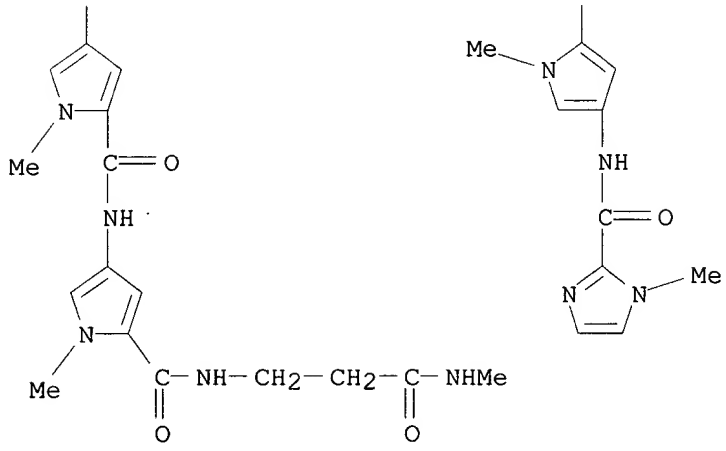

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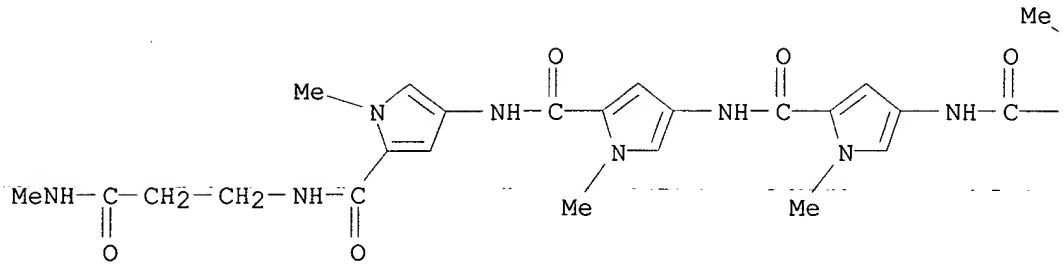

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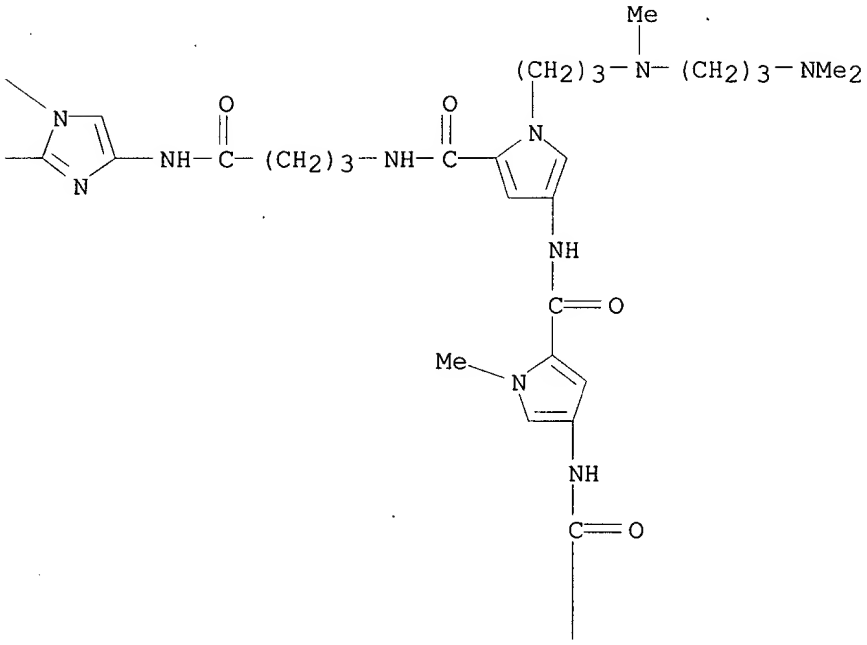

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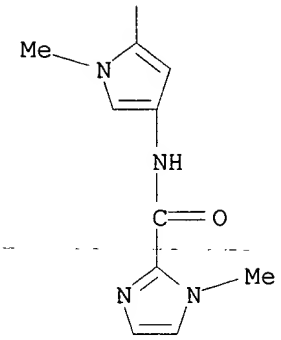

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(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
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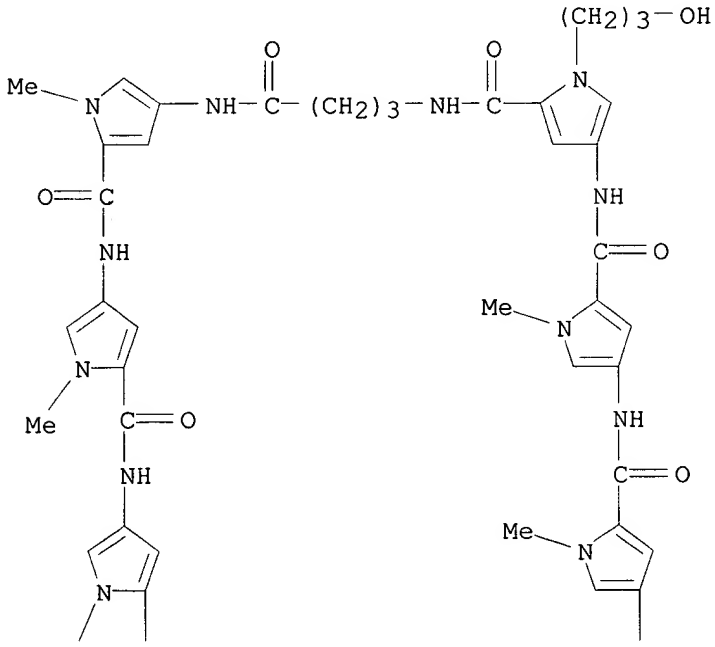

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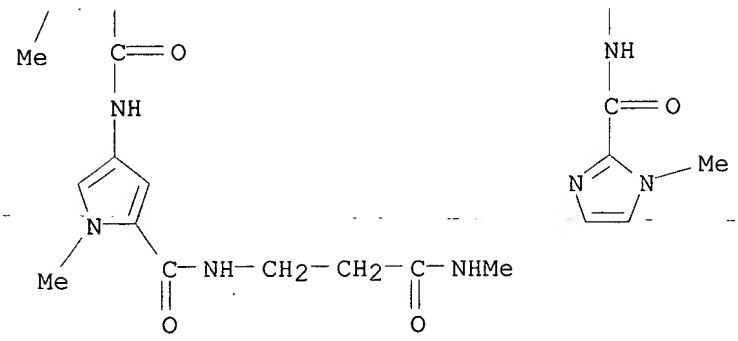

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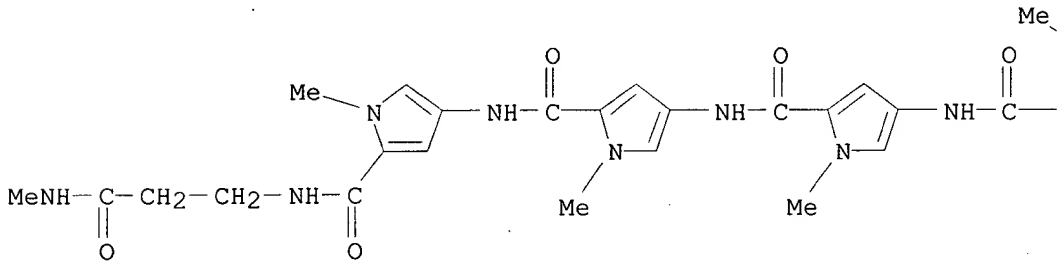

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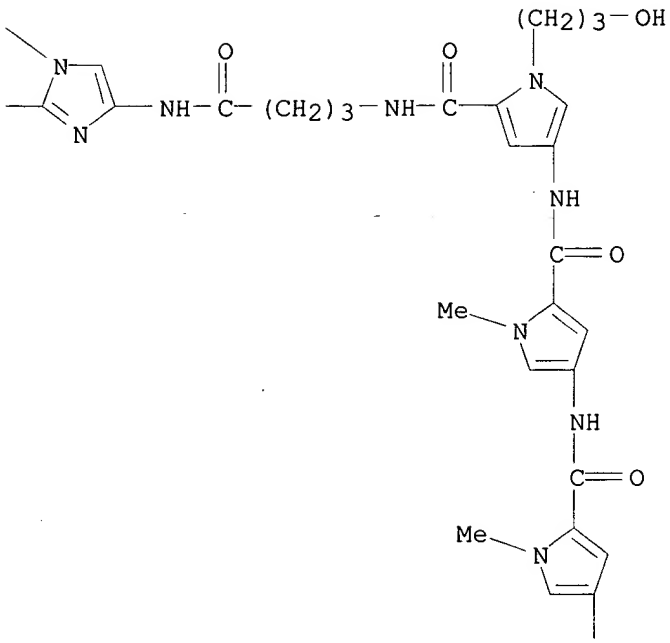

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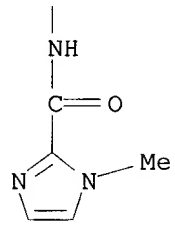
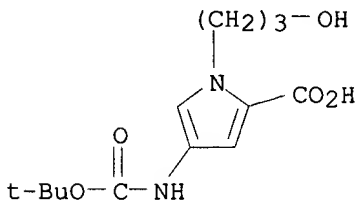


IT **374694-42-5**
RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
RN 374694-42-5 HCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-(3-hydroxypropyl)- (9CI) (CA INDEX NAME)



IT **5930-92-7 374694-50-5D**, Conjugate with resin
RL: RCT (Reactant); RACT (Reactant or reagent)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
RN 5930-92-7 HCAPLUS
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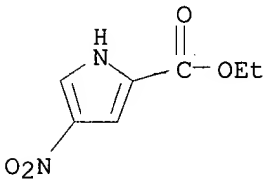

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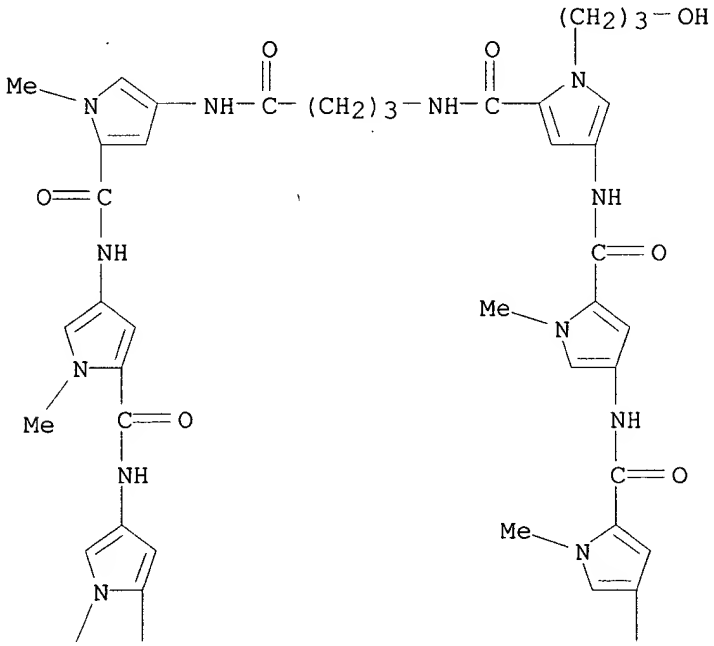

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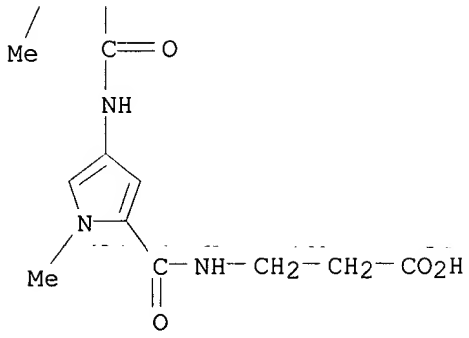

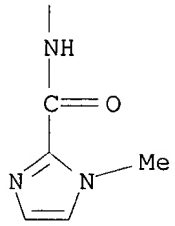

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
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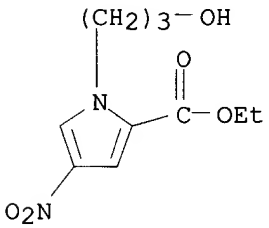


REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> D IND 1

L29 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2002 ACS
CC 6-3 (General Biochemistry)
Section cross-reference(s): 3, 28
ST DNA bZIP GCN4 binding inhibition **polyamide** prepn transcriptional regulation
IT Transcription factors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(GCN4; inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
IT Protein motifs
(bZIP domain; inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
IT Proteins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(bZIP-contg.; inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
IT Transcriptional regulation
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
IT **Polyamides**, biological studies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
IT DNA
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
IT **180530-17-0 180530-18-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
IT **374694-23-2P 374694-25-4P 374694-27-6P**
374694-30-1P 374694-32-3P 374694-35-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
IT **374694-45-8P 374694-47-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
IT 191916-06-0D, Self complementary duplex 374733-55-8
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)
IT **374694-42-5**
RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)

IT **5930-92-7 374694-50-5D**, Conjugate with resin
RL: RCT (Reactant); RACT (Reactant or reagent)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)

IT **374694-40-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(inhibition of major groove DNA binding bZIP proteins by pos. patch **polyamides**)

=> d ibib abs hitstr 2

L29 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:330368 HCAPLUS
TITLE: Is HCN polymer the primordial biopolymer?.
AUTHOR(S): Minard, Robert D.
CORPORATE SOURCE: Chemistry Department, Penn State University, University Park, PA, 16802, USA
SOURCE: Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, 2000 (2000), GEOC-056. American Chemical Society: Washington, D. C. CODEN: 69CLAC
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB In spite of impressive successes in 1) the synthesis of many key building blocks for the origin of life and 2) the discovery of the RNA world with its potential for directed mol. evolution, no reasonable and robust chemistries have been discovered for assembling the first self-replicating biopolymer. Recent work has shown that HCN polymers contain both **polyamide** and purine/pyrimidine domains. [Minard, R.D., Hatcher, P.G., Gourley, C.R., and Matthews, C.N. Structural Investigations of Hydrogen Cyanide Polymers: New Insights Using TMAH Thermochemolysis/GC-MS, Origins of Life and the Evol. Of the Biosphere,28:461-473 (1998)] We also now know that a sugar **phosphate backbone** is not essential for nucleic acid base-pairing chem. Is it possible that that HCN polymer, formed in large quantities under yet-to-be-detd. "right" conditions, could be the primordial biopolymer first capable of replication and which ultimately led to the RNA world This question will be examd.

=> d ibib abs hitstr 3

L29 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:188887 HCAPLUS
DOCUMENT NUMBER: 132:329537
TITLE: Effects in live cells of a c-myc anti-gene PNA linked to a nuclear localization signal
AUTHOR(S): Cutrona, Giovanna; Carpaneto, Elisabetta M.; Ulivi, Massimo; Roncella, Silvio; Landt, Olfert; Ferrarini, Manlio; Boffa, Lidia C.
CORPORATE SOURCE: Servizi di Immnunologia Clinica, National Cancer Institute, Genoa, Italy
SOURCE: Nature Biotechnology (2000), 18(3), 300-303
CODEN: NABIF9; ISSN: 1087-0156
PUBLISHER: Nature America
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Peptide nucleic acids (PNA) are synthetic homologs of nucleic acids in which the **phosphate**-sugar polynucleotide **backbone** is replaced by a flexible **polyamide**. In this study, a PNA construct was employed as an anti-gene agent in intact cells in culture. The cell lines studied were derived from Burkitt's lymphomas (BL) that presented a translocated and hyperexpressed c-myc oncogene. A 17-mer anti-myc PNA, complementary to a unique sequence located at the beginning of the second exon of the oncogene, and was covalently linked at its N terminus to a nuclear localization signal (NLS) (PNA-mycwt-NLS). When BL cells were exposed to PNA-mycwt-NLS, the anti-gene construct was localized predominantly in the cell nuclei and a rapid consequent down-regulation of c-myc expression occurred. Under these conditions, both completion of a productive cell cycle and apoptosis were inhibited.
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 4

L29 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:112744 HCAPLUS
DOCUMENT NUMBER: 132:318974
TITLE: Conformational Flexibility of B-DNA at 0.74 .ANG. Resolution: d(CCAGTACTGG)2
AUTHOR(S): Kielkopf, Clara L.; Ding, Sheng; Kuhn, Peter; Rees, Douglas C.
CORPORATE SOURCE: Division of Biology, California Inst. Technol., Pasadena, CA, USA
SOURCE: Journal of Molecular Biology (2000), 296(3), 787-801
CODEN: JMOBAK; ISSN: 0022-2836
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The affinity and specificity of a ligand for its DNA site is a function of the conformational changes between the isolated and complexed states. Although the structures of a hydroxypyrrole-imidazole-pyrrole **polyamide** dimer with 5'-CCAGTACTGG-3' and the trp repressor recognizing the sequence 5'-GTACT-3' are known, the baseline conformation of the DNA site would contribute to our understanding of DNA recognition by these ligands. The 0.74 .ANG. resoln. structure of a B-DNA double helix, 5'-CCAGTACTGG-3', has been detd. by x-ray crystallog. Six of the nine **phosphates**, two of four bound calcium ions and networks of water mols. hydrating the oligonucleotide have alternate conformations. By contrast, nine of the ten bases have a single, unique conformation with hydrogen atoms visible in most cases. The **polyamide** mols. alter the geometry of the **phosphodiester backbone**, and the water mols. mediating contacts in the trp repressor/operator complex are conserved in the unliganded DNA. Furthermore, the multiple conformational states, ions and hydration revealed by this ultrahigh resoln. structure of a B-form oligonucleotide are potentially general considerations for understanding DNA-binding affinity and specificity by ligands. (c) 2000 Academic Press.
REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> D IND 4

L29 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2002 ACS
CC 6-2 (General Biochemistry)
ST DNA conformation calcium binding
IT Conformation
(DNA; conformational flexibility of d(CCAGTACTGG)2 B-DNA at 0.74 .ANG. resoln.)
IT 7440-70-2, Calcium, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(DNA binding)
IT 195841-32-8
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(conformational flexibility of d(CCAGTACTGG)2 B-DNA at 0.74 .ANG. resoln.)

=> d ibib abs hitstr 5

L29 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:618936 HCAPLUS
DOCUMENT NUMBER: 129:227036
TITLE: Peptide nucleic acids (PNA) and PNA-DNA chimeras. From high binding affinity towards biological function
AUTHOR(S): Uhlmann, Eugen
CORPORATE SOURCE: Hoechst Marion Roussel Deutschland G.m.b.H., Frankfurt/Main, D-65926, Germany
SOURCE: Biological Chemistry (1998), 379(8/9), 1045-1052
CODEN: BICHF3; ISSN: 1431-6730
PUBLISHER: Walter de Gruyter & Co.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review is given with 45 refs. Oligonucleotide analogs are of major interest as tools in mol. biol., as diagnostics, and as potential pharmaceuticals which bind in a predictable way to certain nucleic acid target sequences, aiming at the inhibition of expression of disease-causing genes. One of the most promising nucleic acid mimetics are the peptide- or **polyamide**- nucleic acids (PNA) which bind with higher affinity to DNA and RNA than natural oligonucleotides. In these non-ionic PNAs, the entire sugar-**phosphate backbone** is replaced by an N-amino-ethylglycine-based **polyamide** structure. A unique property of PNA is its ability to displace one strand of a DNA double-helix. This strand displacement process, which is inefficient with DNA, is supported by the formation of an unusually stable internal (PNA), DNA triple helix. The combination of PNA and DNA in 1 mol. results in PNA/DNA chimeras with new properties. They show improved aq. soly. compared to pure PNAs due to their partially neg. charged structure. The cellular uptake of the chimeras is better than of pure PNAs. In contrast to PNA, the chimeras bind exclusively in the antiparallel orientation under physiol. conditions. The binding affinity is generally stronger when the PNA/DNA chimeras are hybridized to RNA than to DNA, whereby the strength of binding strongly depends on the PNA: DNA ratio. PNA/DNA chimeras are recognized as substrates by various nucleic acid processing enzymes, and consequently can also assume biol. functions, such as a primer function for DNA polymerases. Pure PNA cannot induce RNase H cleavage of target RNA, which is believed to support the biol. efficacy of antisense agents. DNA-PNA chimeras are able to stimulate cleavage of the target RNA by RNase H upon formation of an RNA chimera duplex.

=> d ibib abs hitstr 6

L29 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:604922 HCAPLUS
DOCUMENT NUMBER: 129:198864
TITLE: Inhibition of major groove DNA binding proteins by minor groove-binding **polyamides** containing major groove-directed positive charge
INVENTOR(S): Baird, Eldon E.; Dervan, Peter B.
PATENT ASSIGNEE(S): California Institute of Technology, USA
SOURCE: PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 10
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9837087	A1	19980827	WO 1998-US2684	19980213
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, US, US, US, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6090947	A	20000718	US 1996-607078	19960226
US 6143901	A	20001107	US 1997-837524	19970421
AU 9861588	A1	19980909	AU 1998-61588	19980213
EP 973798	A1	20000126	EP 1998-906343	19980213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002514205	T2	20020514	JP 1998-536723	19980213

PRIORITY APPLN. INFO.:

US 1996-607078	A2	19960226
US 1997-43444P	P	19970408
US 1997-42022P	P	19970416
US 1997-837524	A2	19970421
US 1997-853522	A2	19970508
US 1996-23309P	P	19960731
US 1996-24374P	P	19960801
US 1996-26713P	P	19960925
US 1997-38384P	P	19970214
WO 1997-US3332	A	19970220
WO 1997-US12722	A	19970721
WO 1998-US2684	W	19980213

AB This invention provides improved **polyamides** comprising a pos. patch for contacting the **phosphate backbone** or major groove of a DNA mol. As such, the improved **polyamides** are capable of inhibiting the function or binding of a DNA-binding protein to a DNA mol. The improved **polyamide** provides for more efficient function of the **polyamide**. Thus, imidazole- and pyrrole-contg. **polyamides** conjugated to RPRRRR prevented GCN4 from binding to its target DNA.

IT **207978-26-5P 207978-30-1P 208053-41-2P**
208053-42-3P 208053-43-4P 208053-44-5P
208053-45-6P 208053-46-7P 208053-47-8P

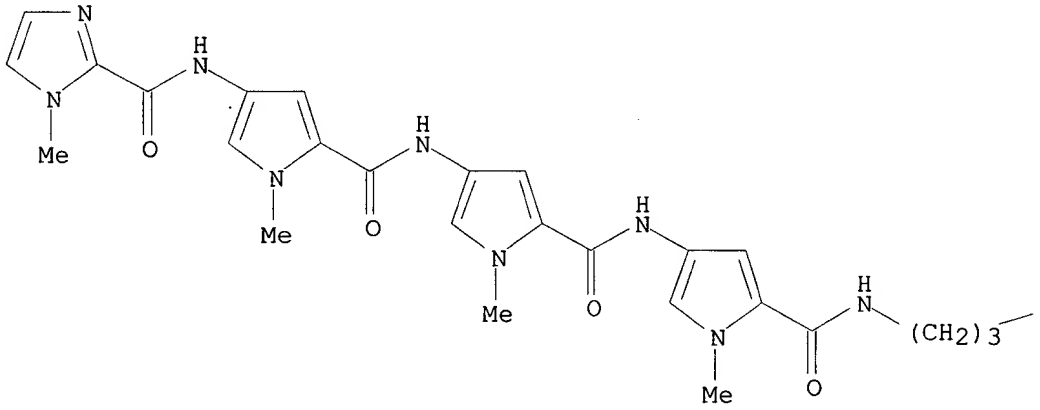
208053-48-9P 208053-49-0P 208053-50-3P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(inhibition of major groove DNA binding proteins by minor groove-binding **polyamides** contg. major groove-directed pos. charge)

RN 207978-26-5 HCAPLUS

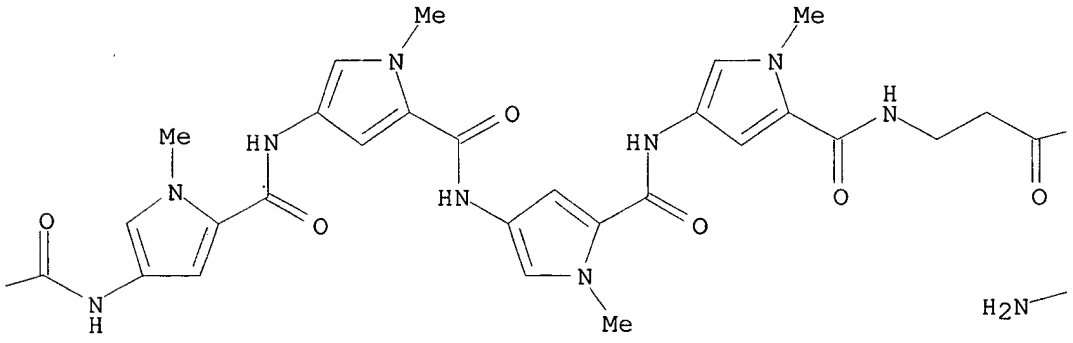
CN L-Argininamide, 1-methyl-1H-imidazole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-aminobutanoyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-.beta.-alanyl-L-arginyl-L-prolyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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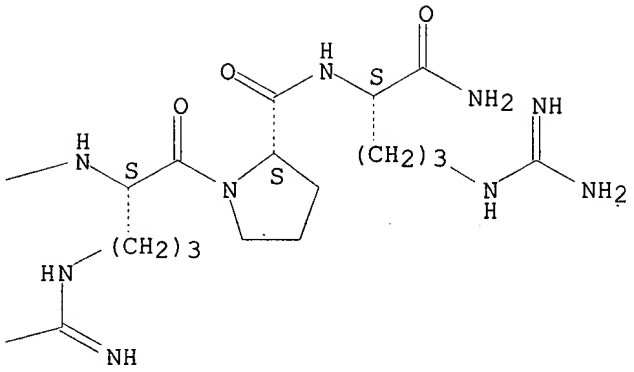

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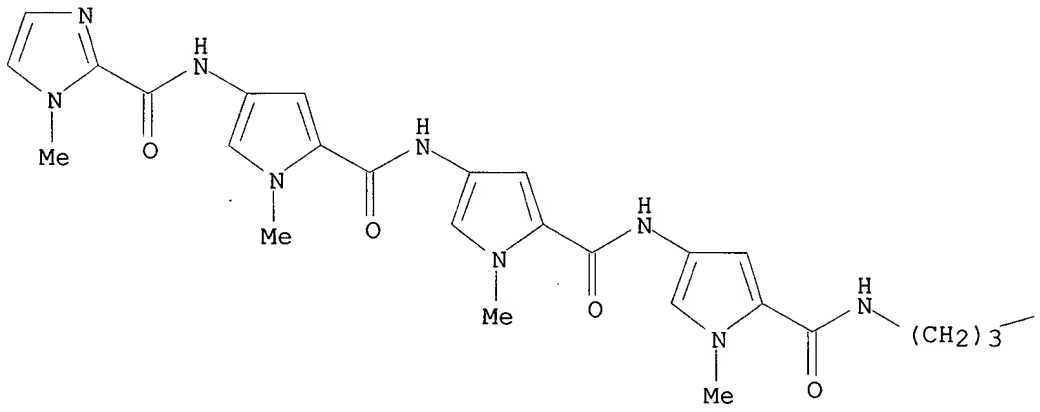
Absolute stereochemistry.

PAGE 1-A



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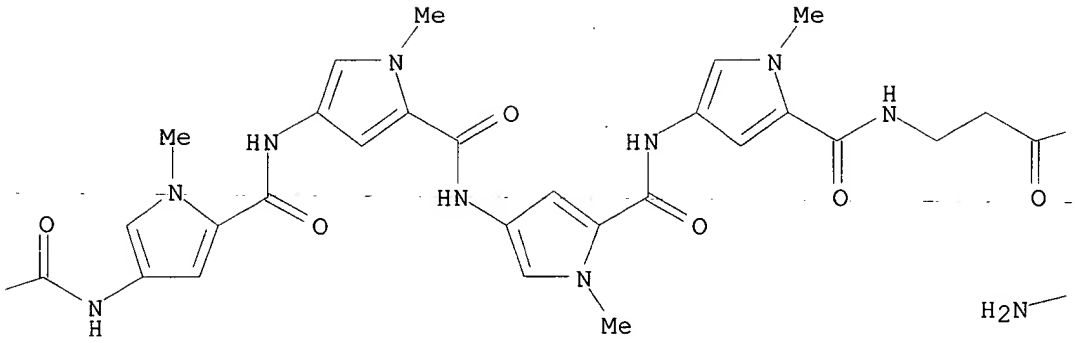

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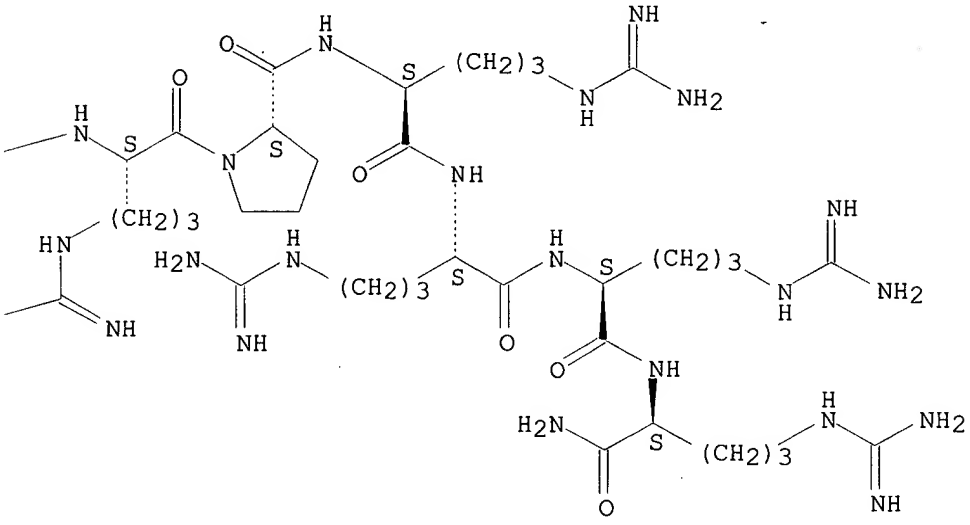

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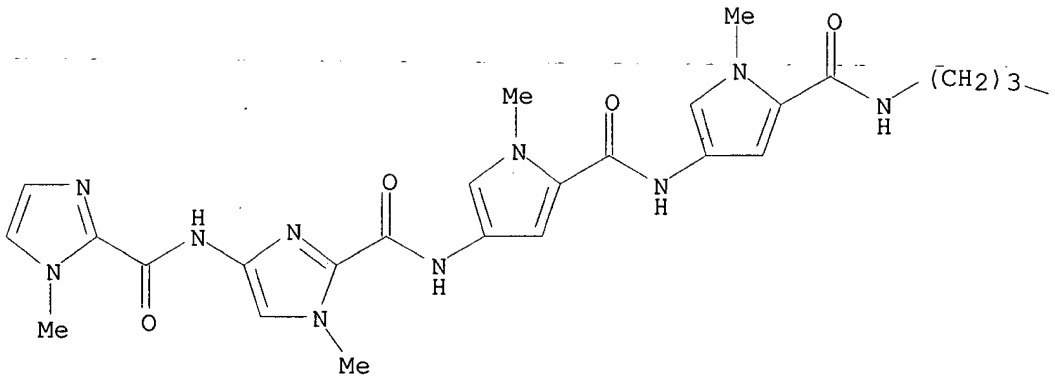
Absolute stereochemistry.

PAGE 1-A



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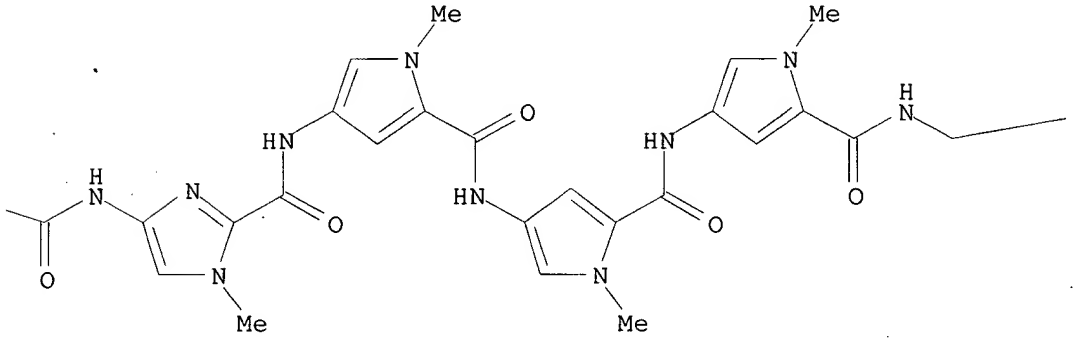

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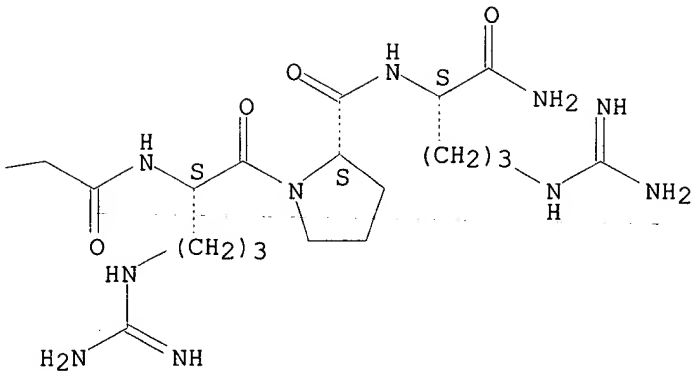

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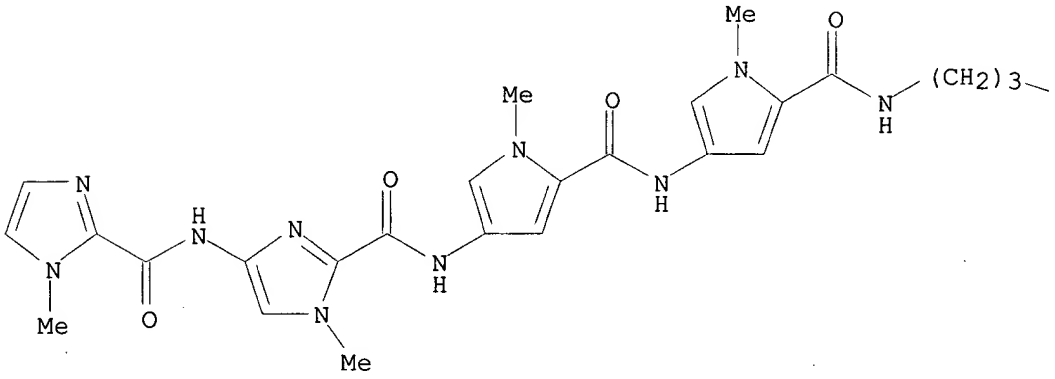
Absolute stereochemistry.

PAGE 1-A



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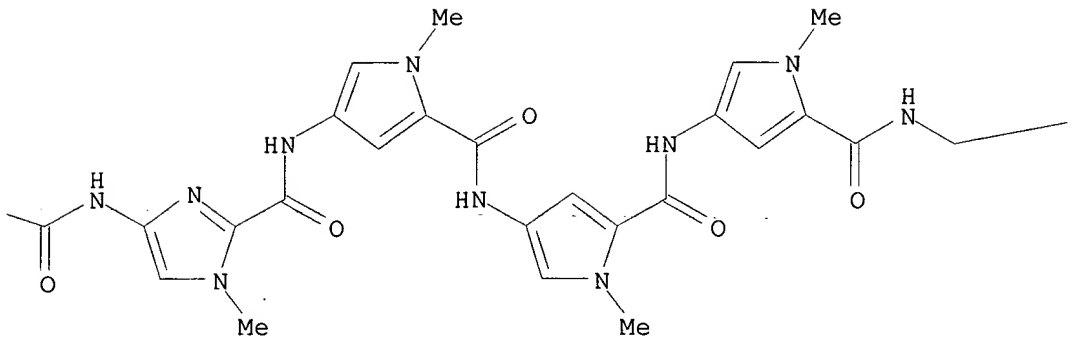

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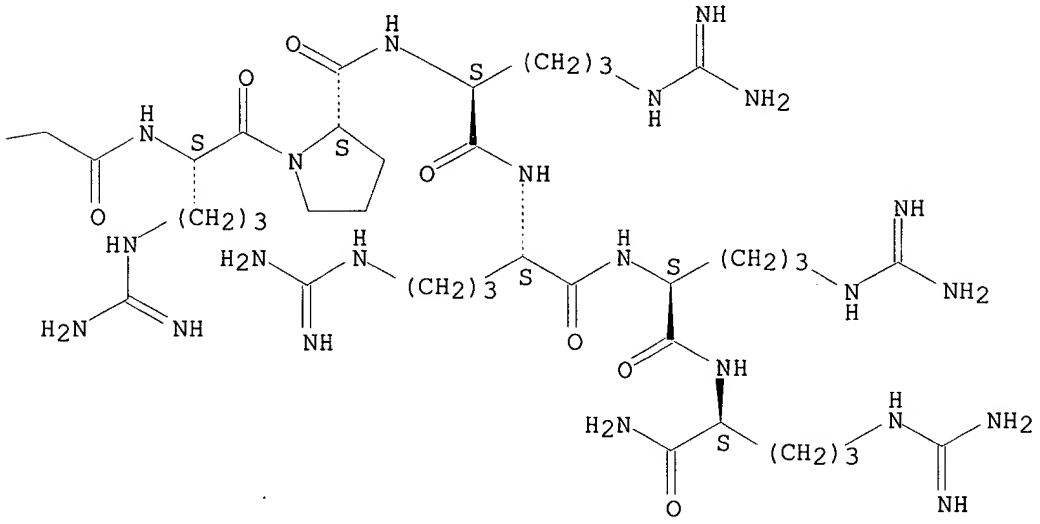

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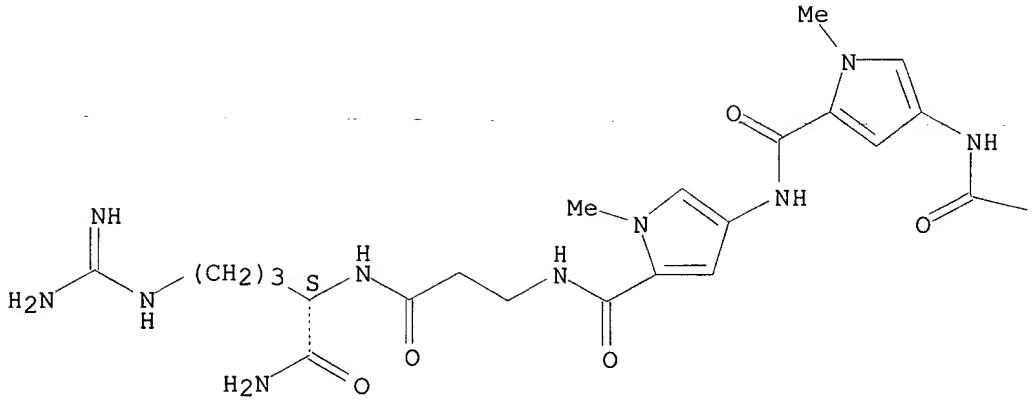
Absolute stereochemistry.

PAGE 1-A



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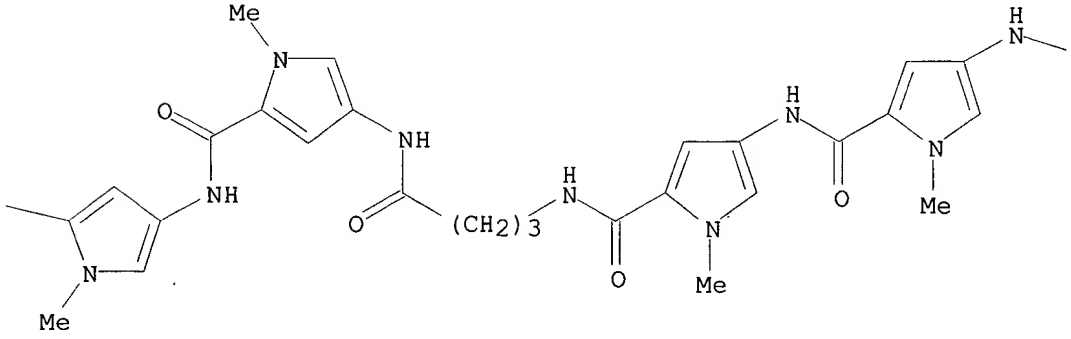

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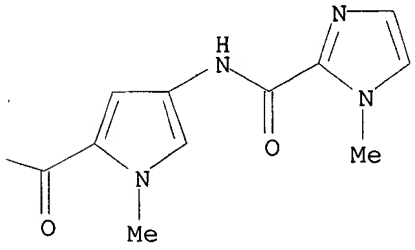

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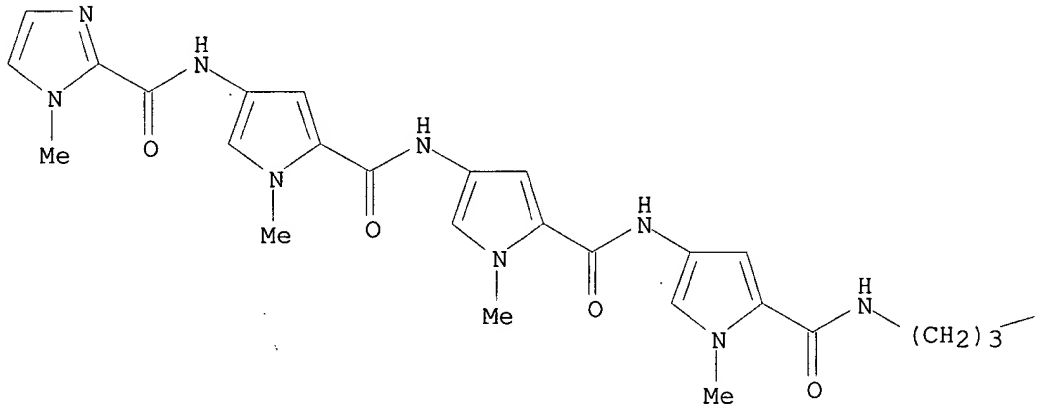
Absolute stereochemistry.

PAGE 1-A



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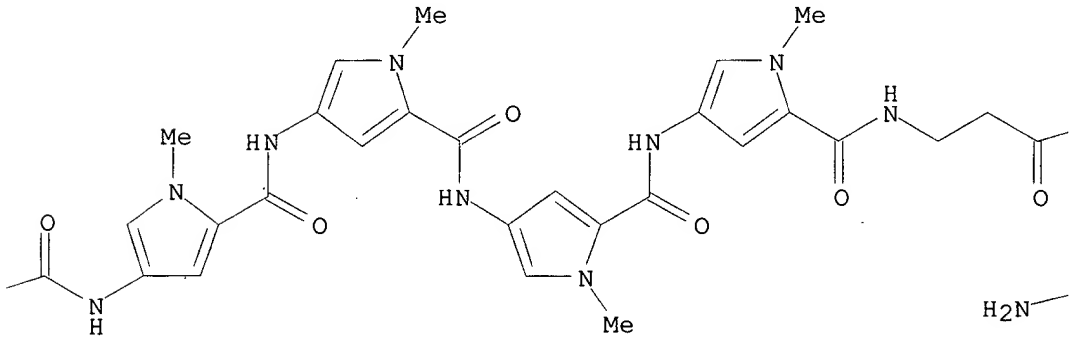

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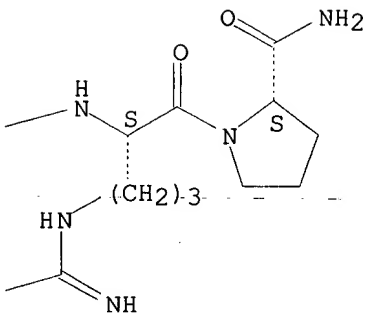

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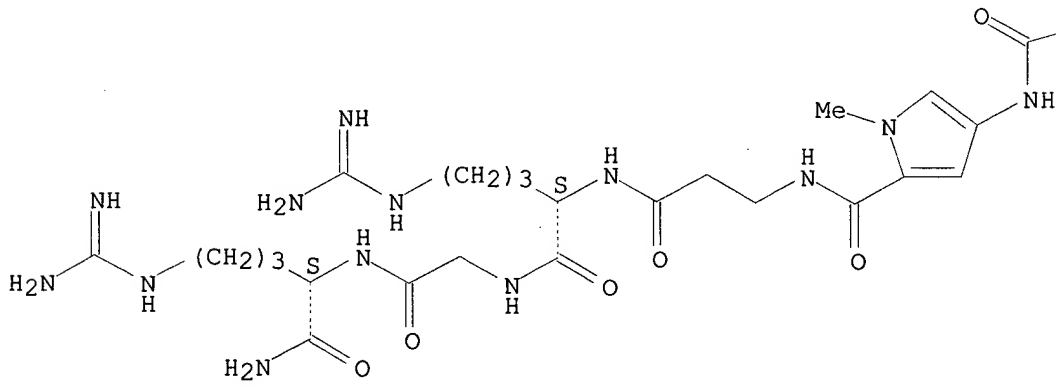
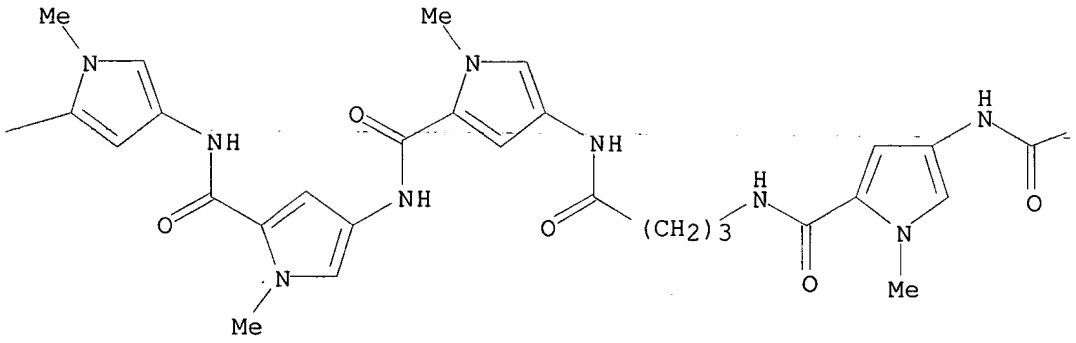
Absolute stereochemistry.

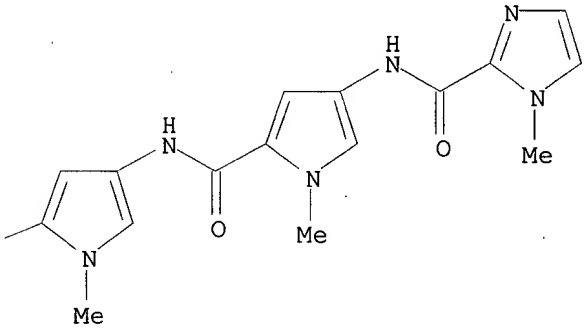
PAGE 1-A



PAGE 1-B



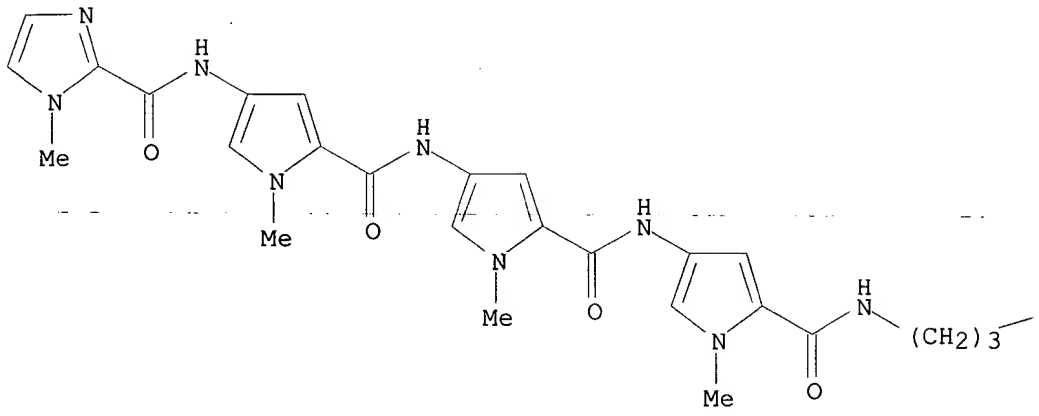
PAGE 1-C



RN 208053-46-7 HCAPLUS
CN L-Argininamide, 1-methyl-1H-imidazole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-aminobutanoyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-.beta.-alanyl-L-arginyl-D-prolyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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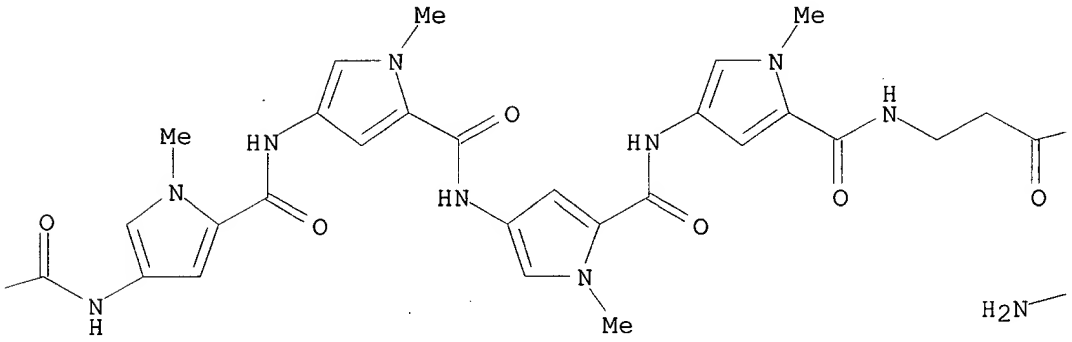
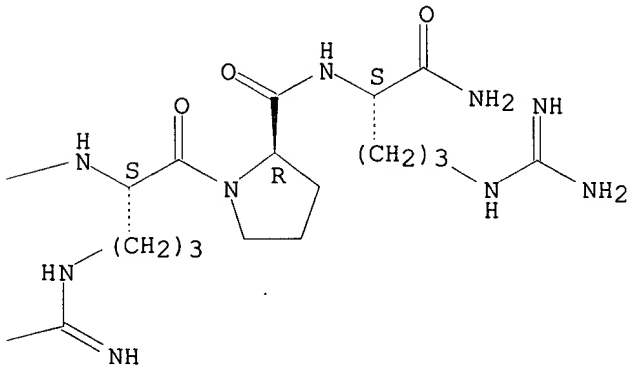


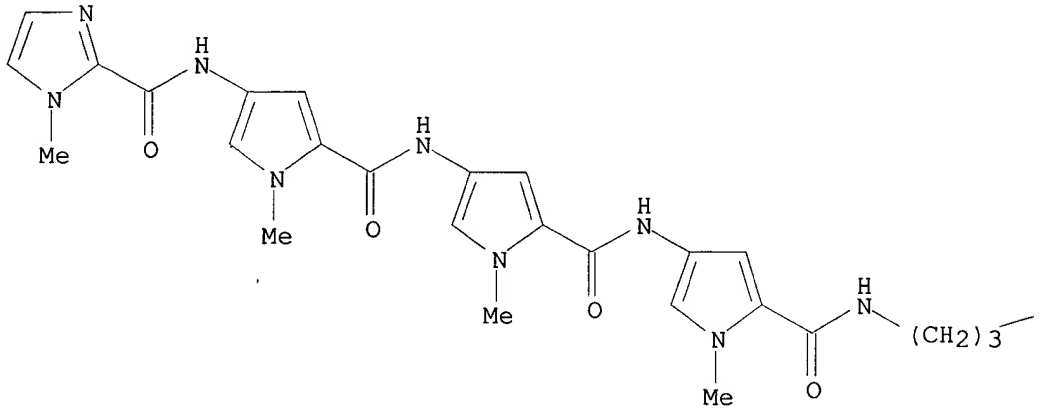
PAGE 1-C



RN 208053-47-8 HCAPLUS
CN L-Argininamide, 1-methyl-1H-imidazole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-aminobutanoyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-.beta.-alanyl-L-alanyl-L-prolyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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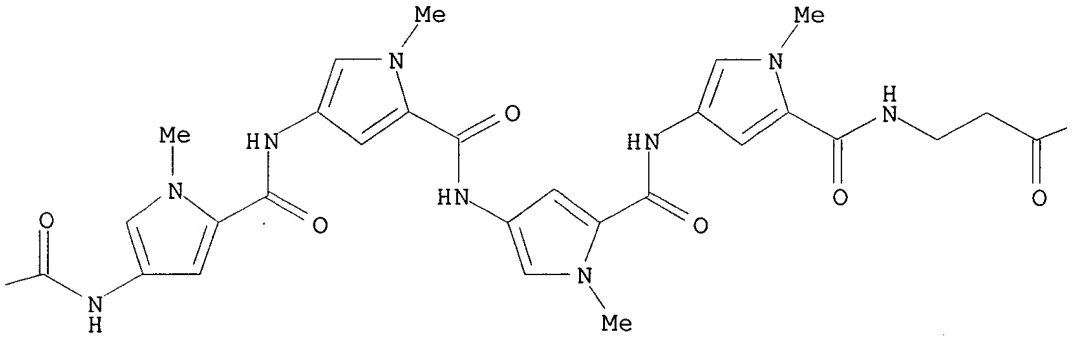
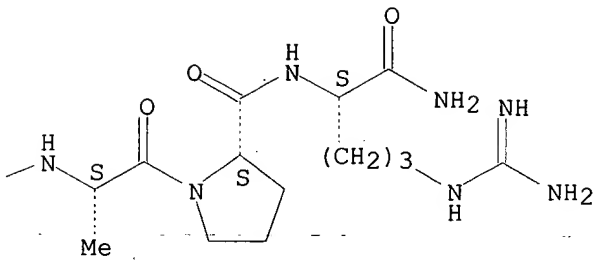


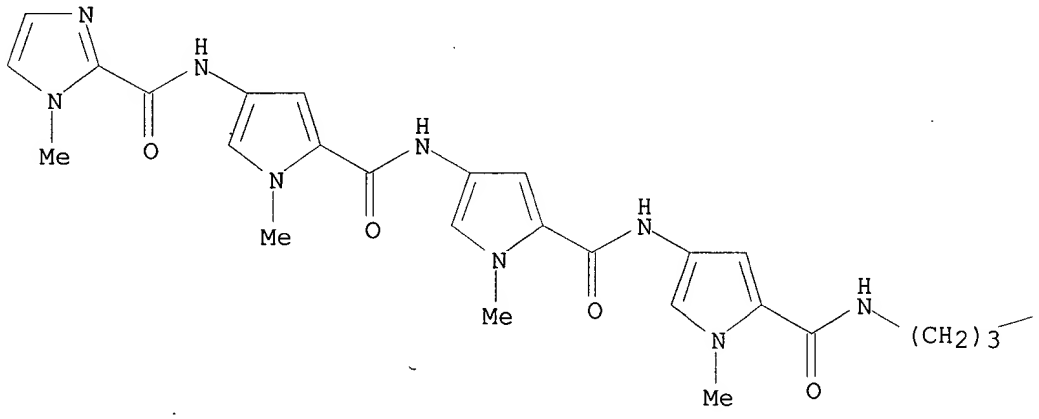
PAGE 1-C



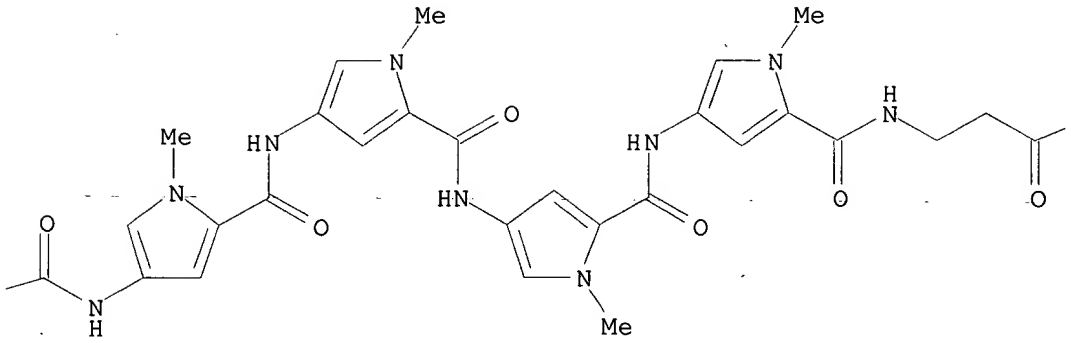
RN 208053-48-9 HCAPLUS
CN L-Argininamide, 1-methyl-1H-imidazole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-aminobutanoyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-.beta.-alanyl-L-lysyl-L-prolyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

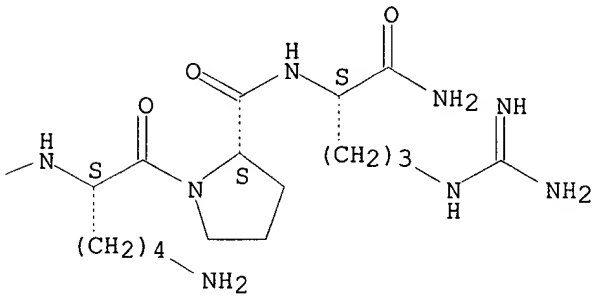
PAGE 1-A



PAGE 1-B



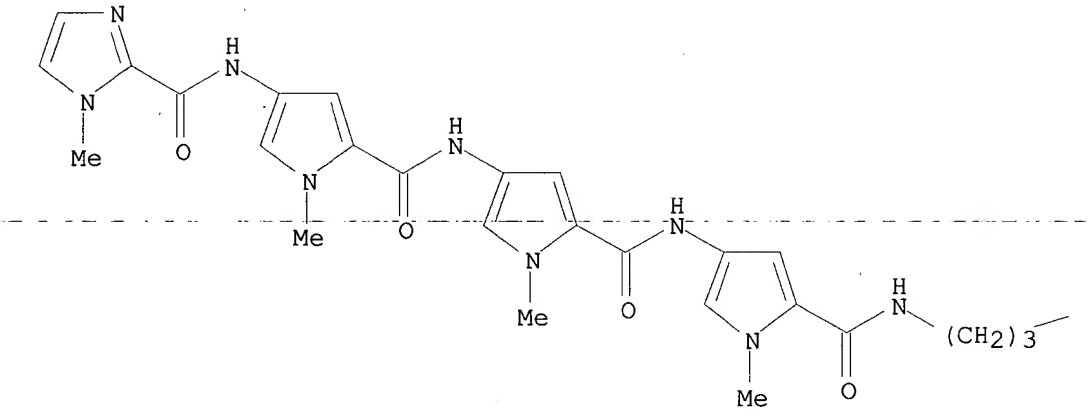
PAGE 1-C



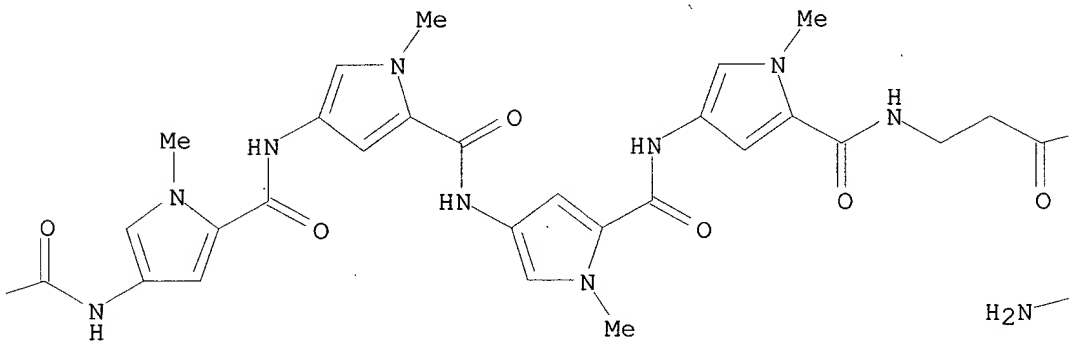
RN 208053-49-0 HCAPLUS
CN L-Lysinamide, 1-methyl-1H-imidazole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-aminobutanoyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-4-amino-1-methyl-1H-pyrrole-2-carbonyl-.beta.-alanyl-L-arginyl-L-prolyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

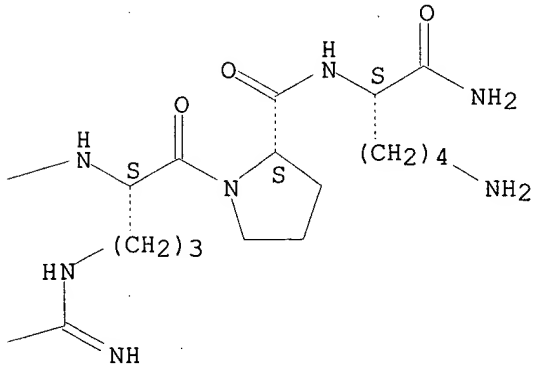
PAGE 1-A



PAGE 1-B



PAGE 1-C



RN 208053-50-3 HCAPLUS
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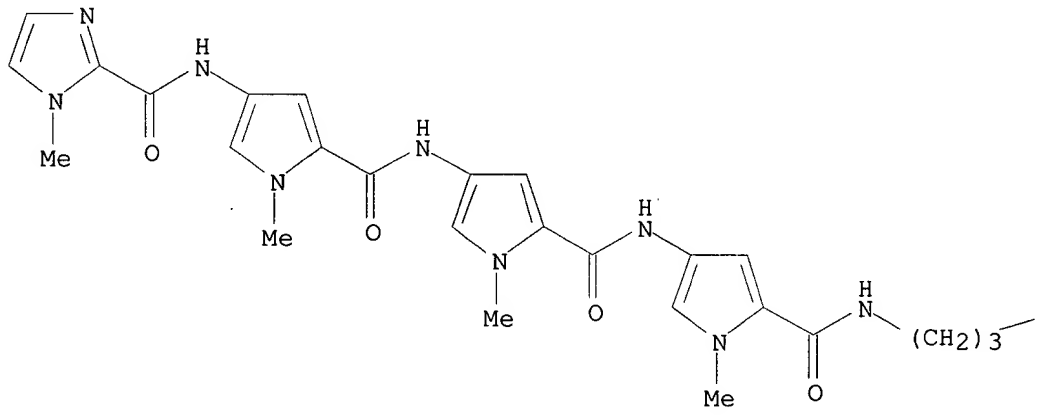
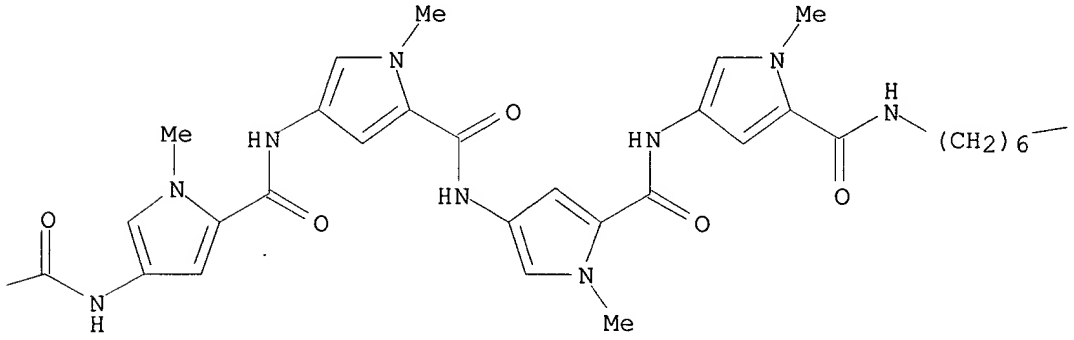
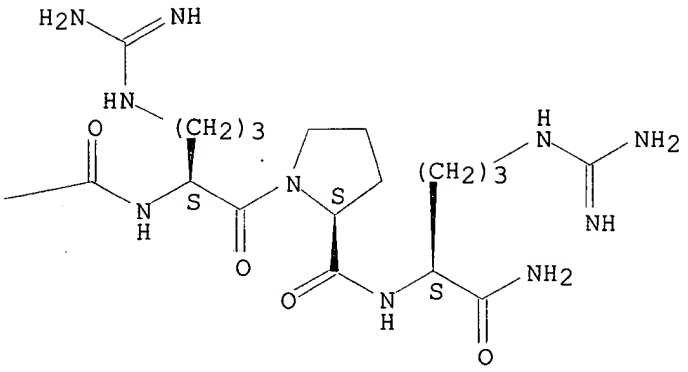
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B





=> D IND 6

L29 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2002 ACS
IC ICM C07K007-02
ICS C07D403-12; A61K038-04; A61K031-415
CC 3-1 (Biochemical Genetics)
ST **polyamide** pyrrole imidazole amino acid contg; DNA binding protein competition **polyamide** conjugate; gene expression regulation **polyamide** conjugate
IT Transcription factors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(GCN4, inhibition of binding to DNA of; inhibition of major groove DNA binding proteins by minor groove-binding **polyamides** contg. major groove-directed pos. charge)
IT Gene
(expression, modulation of; inhibition of major groove DNA binding proteins by minor groove-binding **polyamides** contg. major groove-directed pos. charge)
IT Transcription factors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibition of binding to DNA of; inhibition of major groove DNA binding proteins by minor groove-binding **polyamides** contg. major groove-directed pos. charge)
IT **Polyamides**, biological studies
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(inhibition of major groove DNA binding proteins by minor groove-binding **polyamides** contg. major groove-directed pos. charge)
IT **207978-26-5P 207978-30-1P 208053-41-2P**
208053-42-3P 208053-43-4P 208053-44-5P
208053-45-6P 208053-46-7P 208053-47-8P
208053-48-9P 208053-49-0P 208053-50-3P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(inhibition of major groove DNA binding proteins by minor

groove-binding **polyamides** contg. major groove-directed pos. charge)

=> d ibib abs hitstr 7

L29 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:373255 HCAPLUS
DOCUMENT NUMBER: 129:132651
TITLE: Molecular Dynamics Simulation of a PNA.cntdot.DNA.cntdot.PNA Triple Helix in Aqueous Solution
AUTHOR(S): Shields, George C.; Laughton, Charles A.; Orozco, Modesto
CORPORATE SOURCE: Departament de Bioquimica i Biologia Molecular Facultat de Quimica, Universitat de Barcelona, Barcelona, 08028, Spain
SOURCE: Journal of the American Chemical Society (1998), 120(24), 5895-5904
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mol. dynamics simulations have been used to explore the conformational flexibility of a PNA.cntdot.DNA.cntdot.PNA triple helix in aq. soln. Three 1.05 ns trajectories starting from different but reasonable conformations have been generated and analyzed in detail. All three trajectories converge within about 300 ps to produce stable and very similar conformational ensembles, which resemble the crystal structure conformation in many details. However, in contrast to the crystal structure, there is a tendency for the direct hydrogen-bonds obsd. between the amide hydrogens of the Hoogsteen-binding PNA strand and the **phosphate** oxygens of the DNA strand to be replaced by water-mediated hydrogen bonds, which also involve pyrimidine O2 atoms. This structural transition does not appear to weaken the triplex structure but alters groove widths and so may relate to the potential for recognition of such structures by other ligands (small mols. or proteins). Energetic anal. leads us to conclude that the reason that the hybrid PNA/DNA triplex has quite different helical characteristics from the all-DNA triplex is not because the addnl. flexibility imparted by the replacement of sugar-**phosphate** by PNA **backbones** allows motions to improve base-stacking but rather that base-stacking interactions are very similar in both types of triplex and the driving force comes from weak but definite conformational preferences of the PNA strands.

=> d ibib abs hitstr 8

L29 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:273583 HCAPLUS
DOCUMENT NUMBER: 129:50962
TITLE: Hybridization studies with chiral peptide nucleic acids
AUTHOR(S): Lowe, Gordon; Vilaivan, Tirayut; Westwell, Martin S.
CORPORATE SOURCE: Dyson Perrins Laboratory, Oxford University, Oxford, OX1 3QY, UK
SOURCE: Bioorganic Chemistry (1997), 25(5/6), 321-329
CODEN: BOCMBM; ISSN: 0045-2068
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English

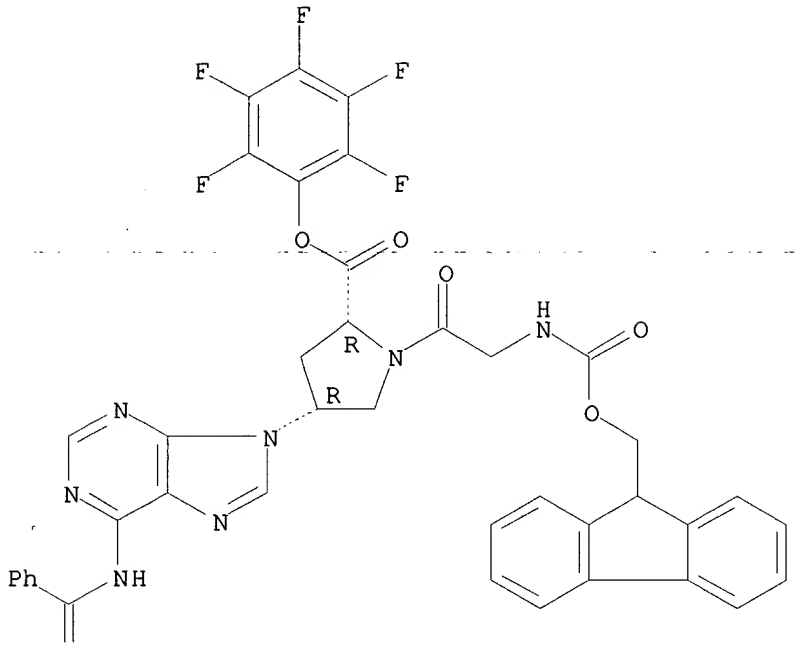
AB A novel class of chiral peptide nucleic acids has been synthesized in which the sugar-**phosphate backbone** of DNA has been replaced with the glycyl-proline backbone of both the L- and the D-configurations, nucleobases being attached through the 4-position of proline with cis- and trans-stereochem. The T10 homopolymers with cis-stereochem. in the L- and D-series bind strongly to poly(dA) with Tm values of 69 and 70.degree., resp. They bind more strongly to poly(rA) with Tm values of 73 and 72.degree., resp., and with apparent 1:1 stoichiometry. Using a mixed sequence decamer it was found that the thermal stability of the chiral peptide nucleic acid/oligonucleotide complex was comparable to that formed by Nielsen's **polyamide** nucleic acid.

IT **189163-58-4 189163-61-9 189163-65-3**
189163-73-3 189163-75-5 189163-77-7
189164-04-3 189164-05-4 189164-06-5
189164-07-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(hybridization studies with chiral peptide nucleic acids)

RN 189163-58-4 HCAPLUS
CN D-Proline, N-[(9H-fluoren-9-ylmethoxy)carbonyl]glycyl-4-[6-(benzoylamino)-9H-purin-9-yl]-, pentafluorophenyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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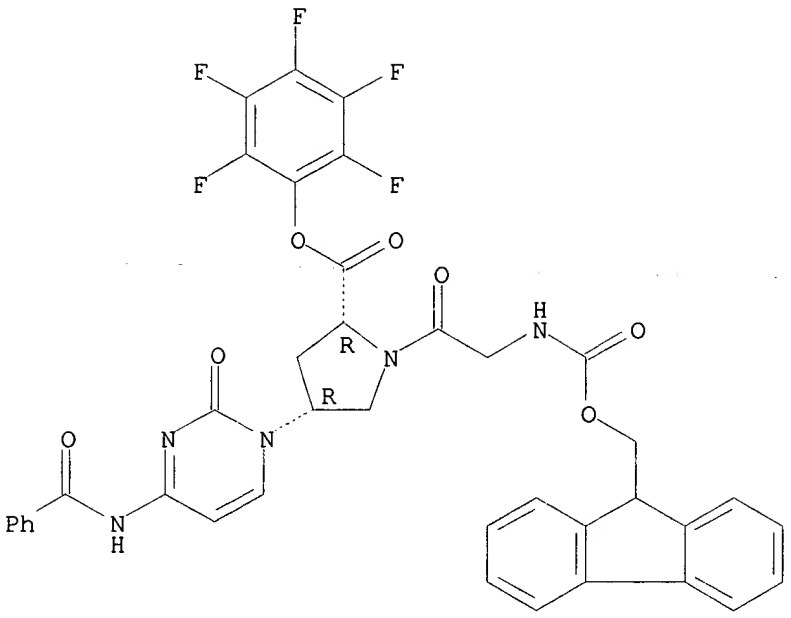
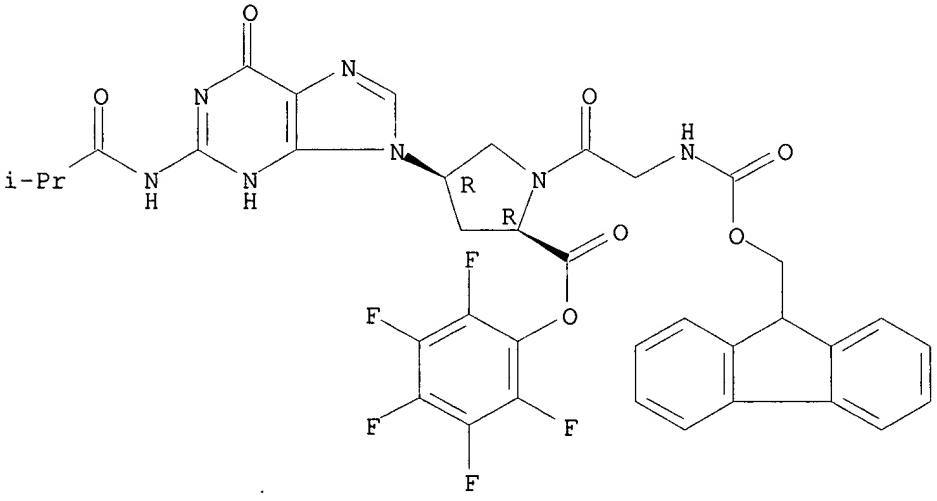
RN 189163-61-9 HCAPLUS
CN D-Proline, N-[(9H-fluoren-9-ylmethoxy)carbonyl]glycyl-4-[4-(benzoylamino)-2-oxo-1(2H)-pyrimidinyl]-, pentafluorophenyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



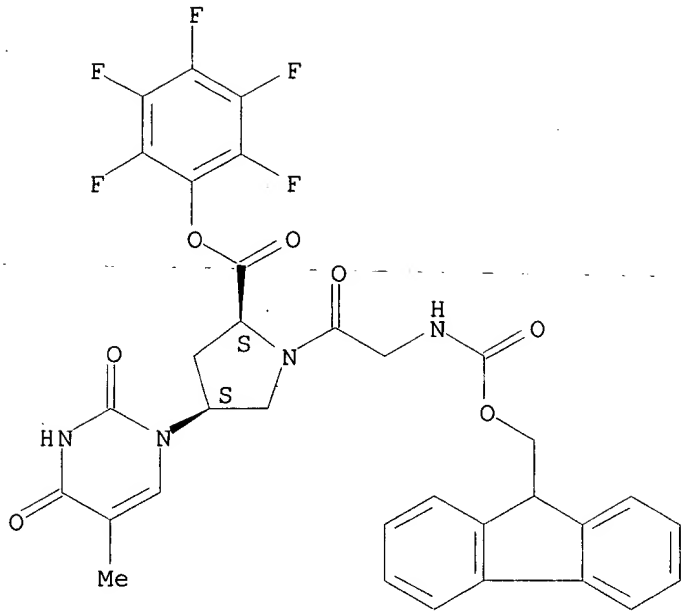
RN 189163-65-3 HCAPLUS
CN D-Proline, N-[(9H-fluoren-9-ylmethoxy)carbonyl]glycyl-4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-9H-purin-9-yl]-, pentafluorophenyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



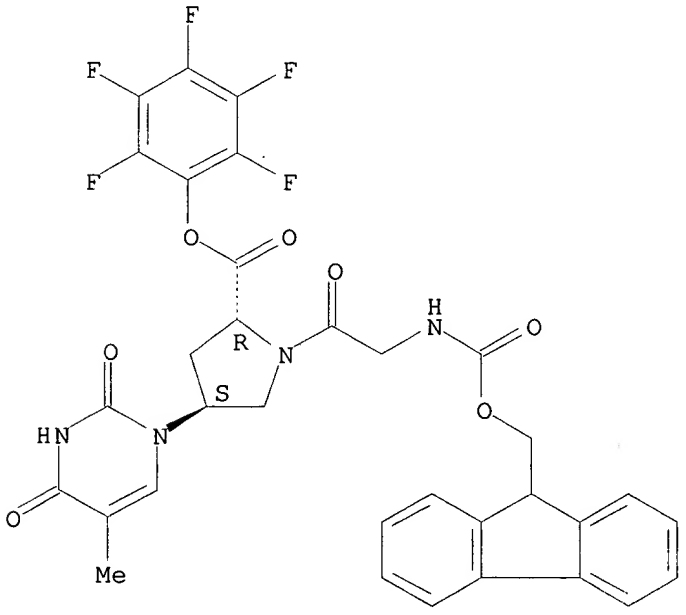
RN 189163-73-3 HCAPLUS
CN L-Proline, N-[(9H-fluoren-9-ylmethoxy)carbonyl]glycyl-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-, pentafluorophenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



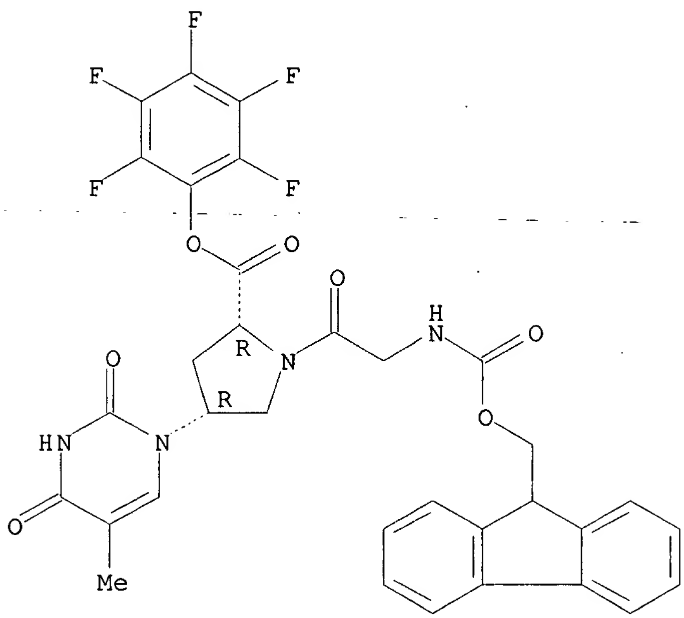
RN 189163-75-5 HCAPLUS
CN D-Proline, N-[(9H-fluoren-9-ylmethoxy)carbonyl]glycyl-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-, pentafluorophenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 189163-77-7 HCAPLUS
CN D-Proline, N-[(9H-fluoren-9-ylmethoxy)carbonyl]glycyl-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-, pentafluorophenyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 189164-04-3 HCAPLUS
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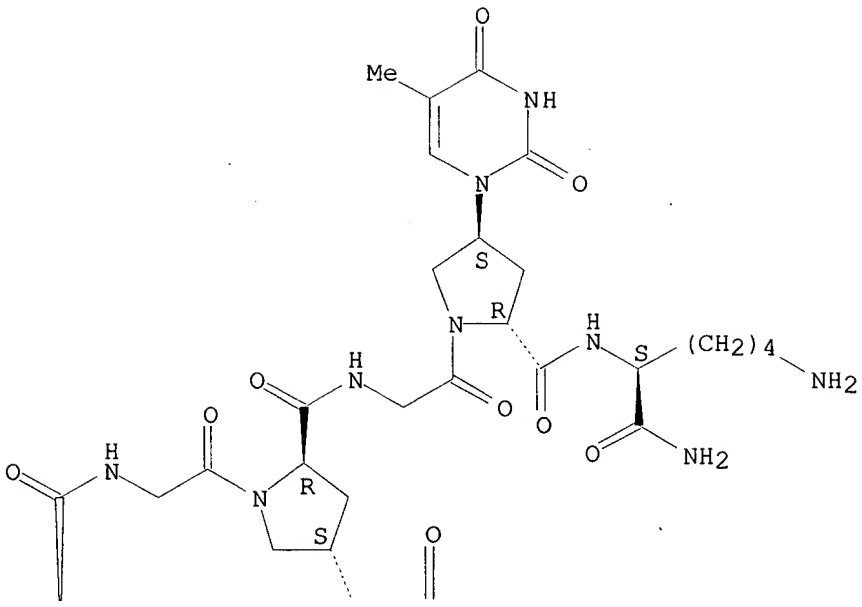
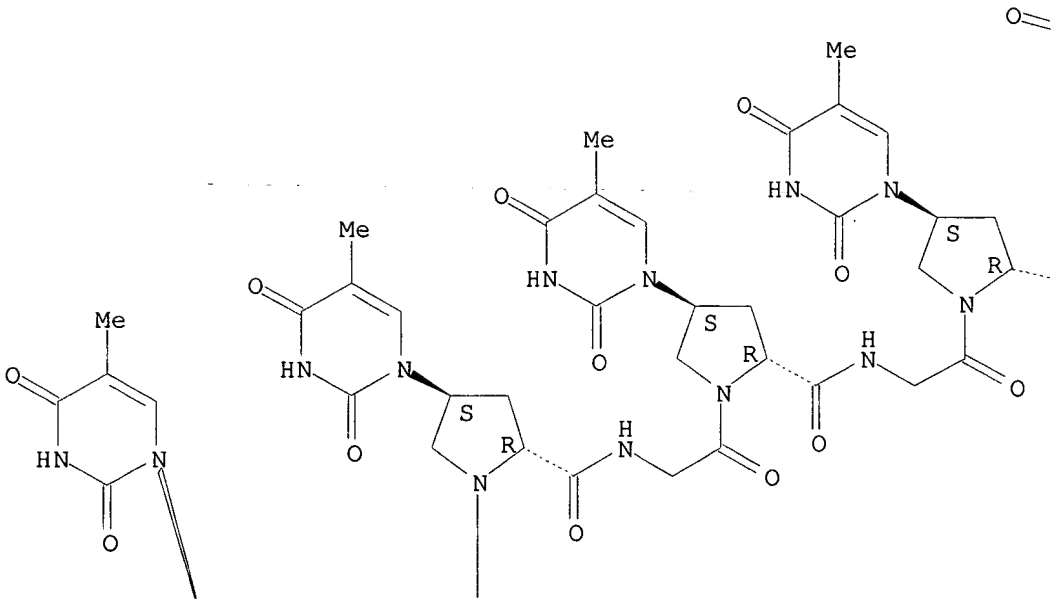
Absolute stereochemistry.

PAGE 1-B

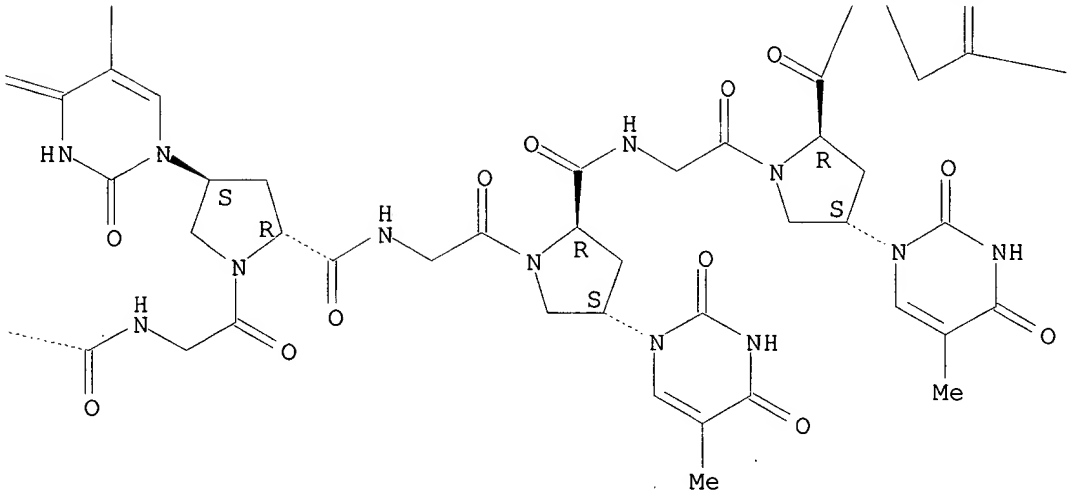
PAGE 1-C



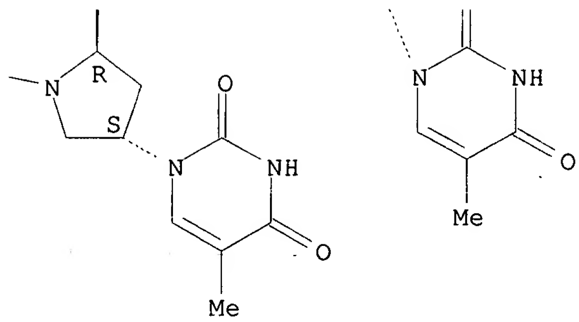
PAGE 2-A



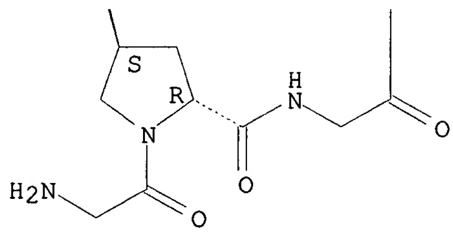
PAGE 2-B



PAGE 2-C



PAGE 3-A

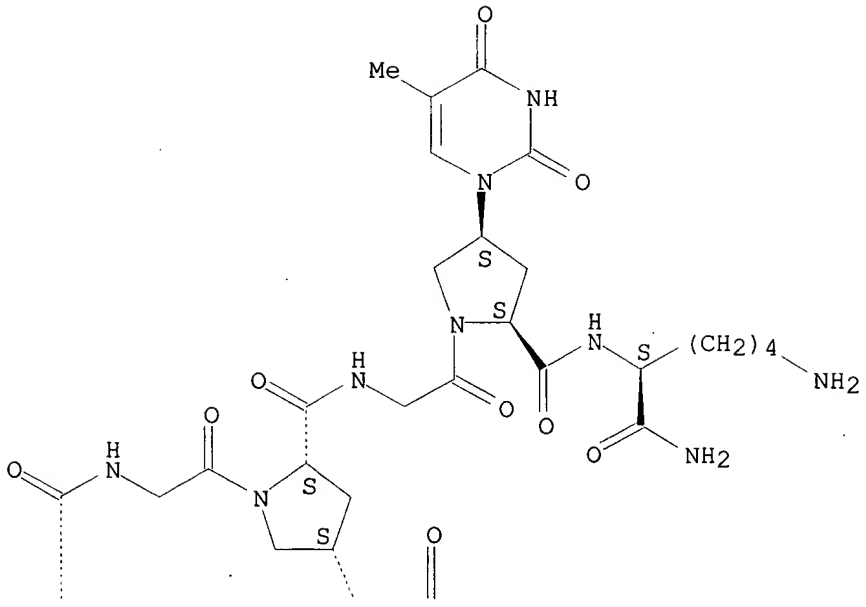


RN 189164-05-4 HCAPLUS
CN L-Lysinamide, glycyl-(4S)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolylglycyl-(4S)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolylglycyl-(4S)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolylglycyl-(4S)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolylglycyl-(4S)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolylglycyl-(4S)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolylglycyl-(4S)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolylglycyl-(4S)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolylglycyl-(4S)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolylglycyl-(4S)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl- (9CI) (CA INDEX NAME)

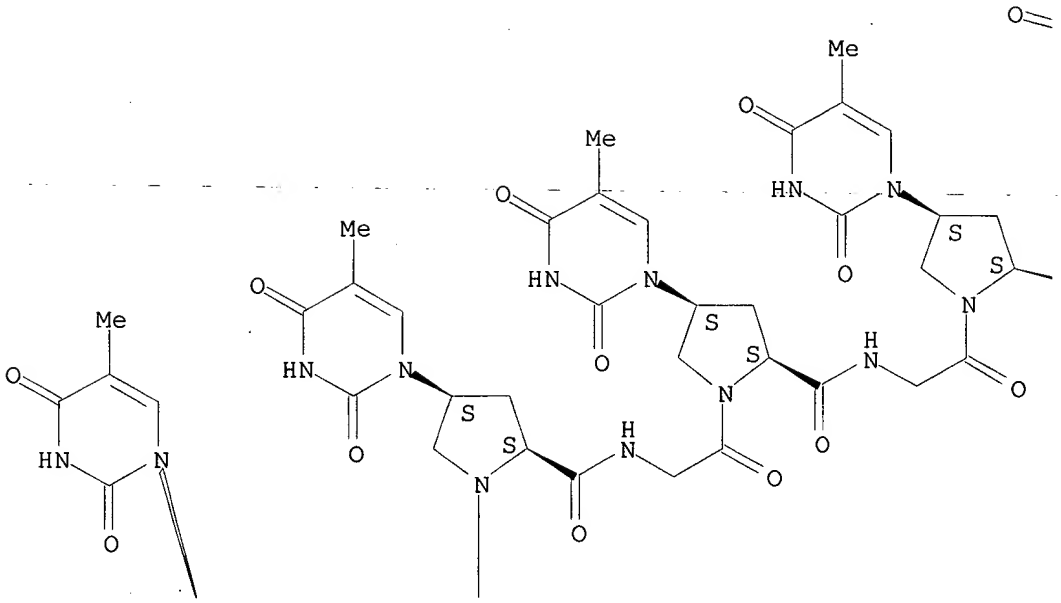
Absolute stereochemistry.

PAGE 1-B

PAGE 1-C



PAGE 2-A



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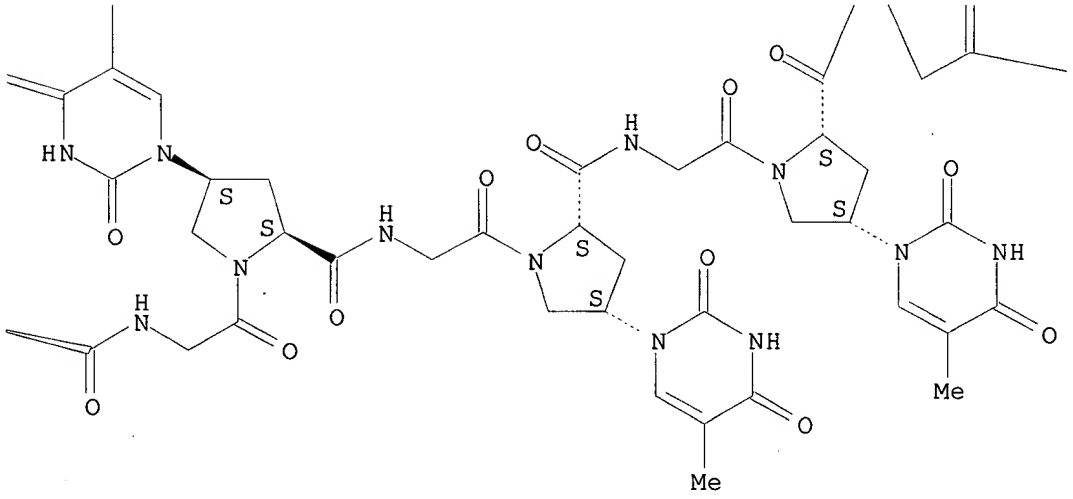
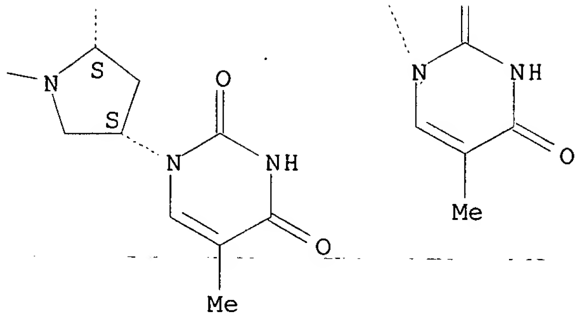
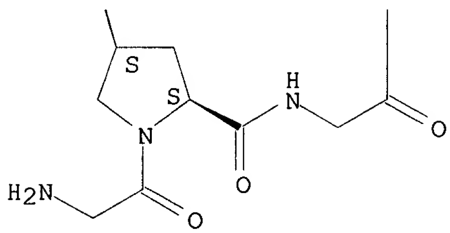


PAGE 2-C



PAGE 3-A

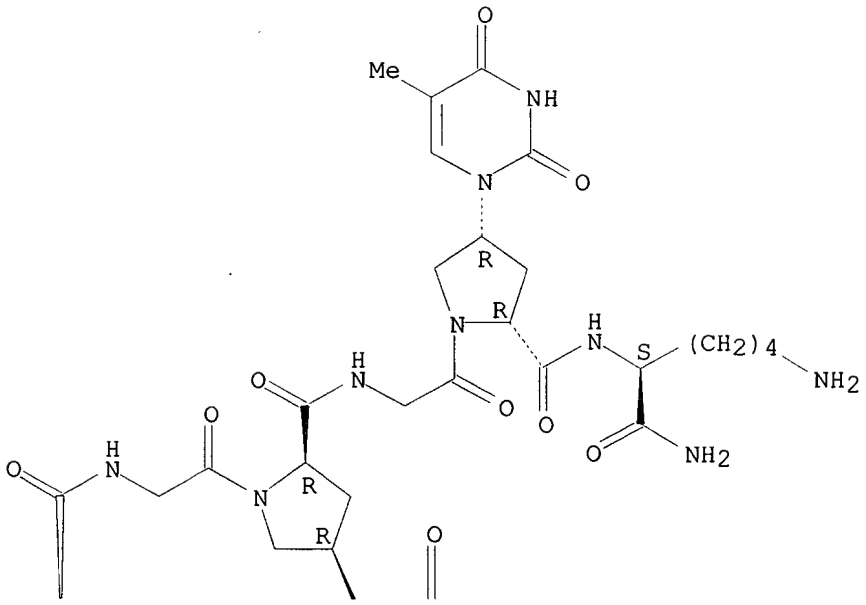


RN 189164-06-5 HCAPLUS
CN L-Lysinamide, glycyl-(4R)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-prolylglycyl-(4R)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-prolylglycyl-(4R)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-prolylglycyl-(4R)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-prolylglycyl-(4R)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-prolylglycyl-(4R)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-prolylglycyl-(4R)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-prolylglycyl-(4R)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-prolylglycyl-(4R)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-prolylglycyl-(4R)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-prolyl- (9CI) (CA INDEX NAME)

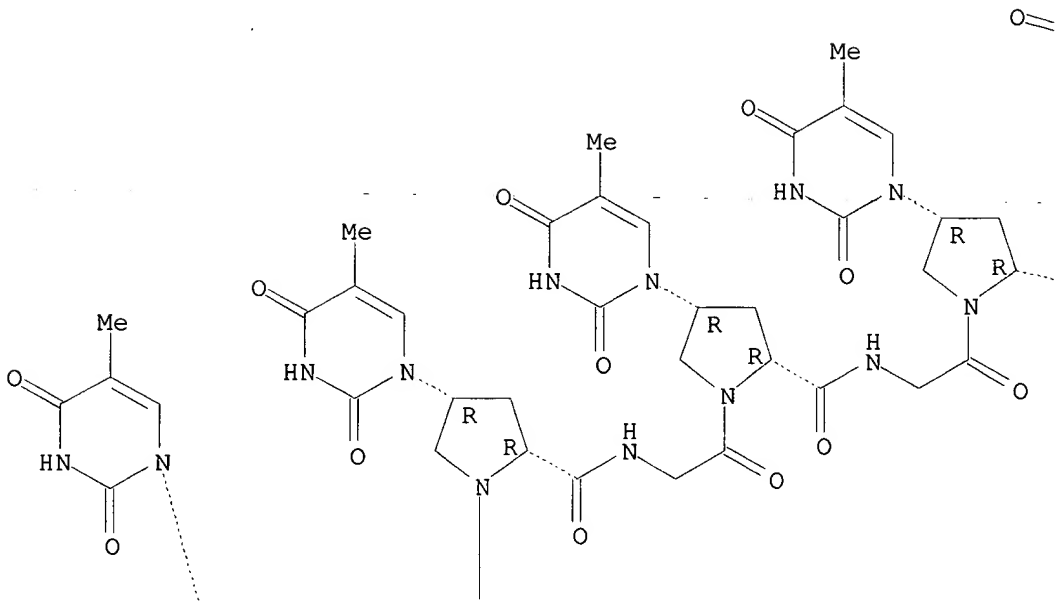
Absolute stereochemistry.

PAGE 1-B

PAGE 1-C



PAGE 2-A



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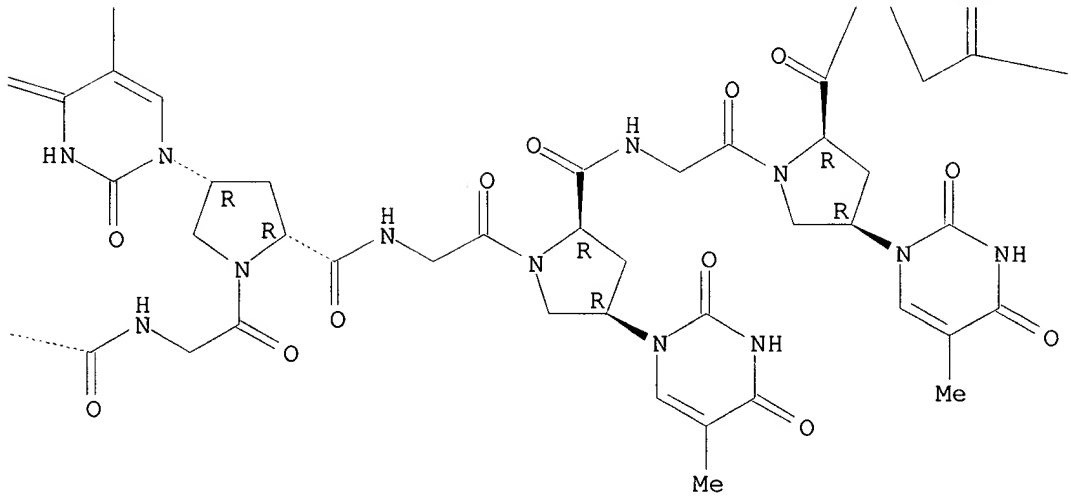

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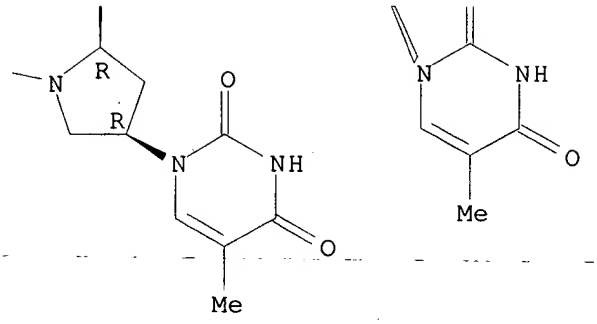
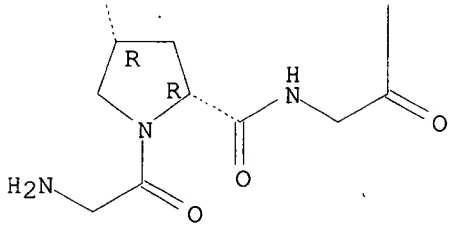


PAGE 3-A



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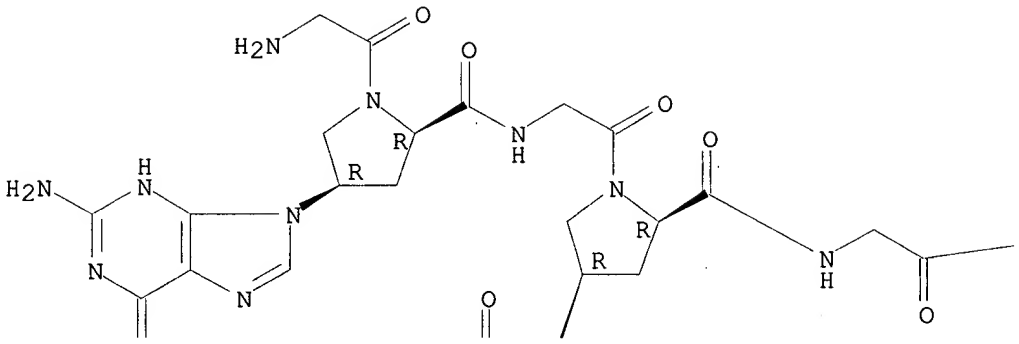
Absolute stereochemistry.

PAGE 1-A



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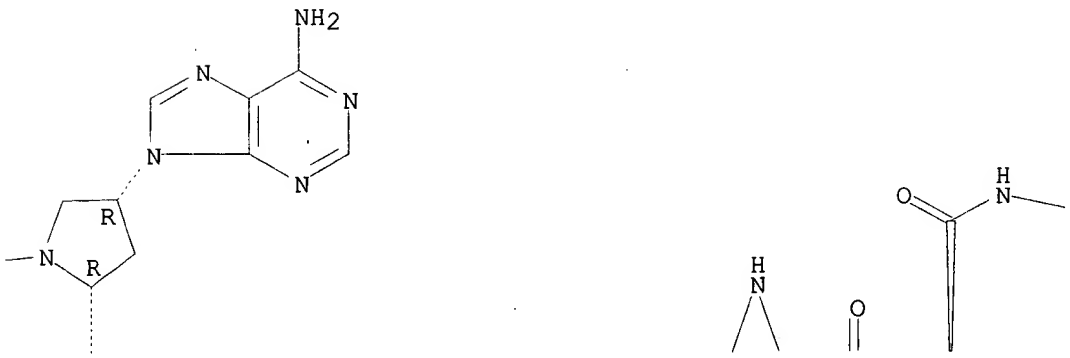

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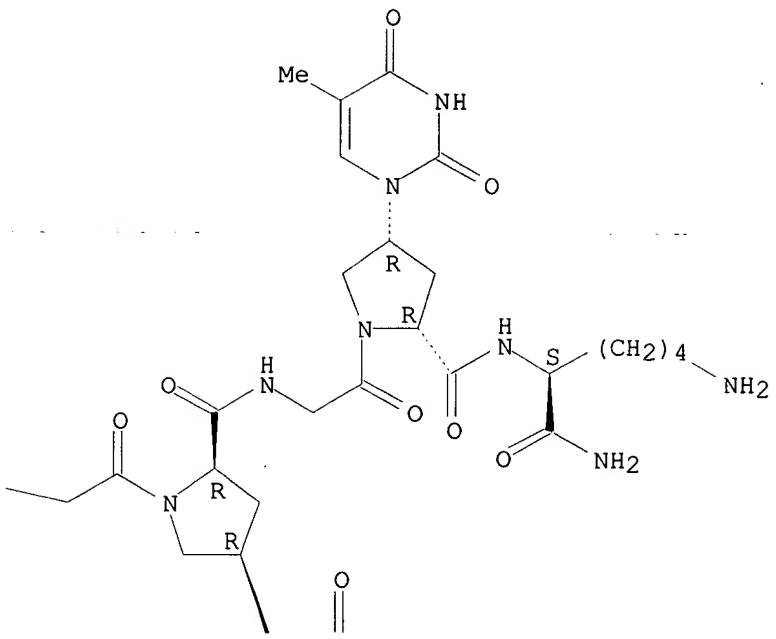

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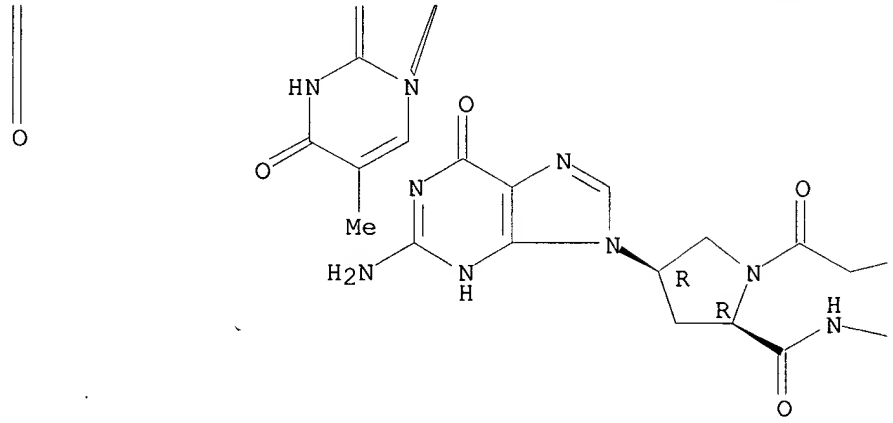

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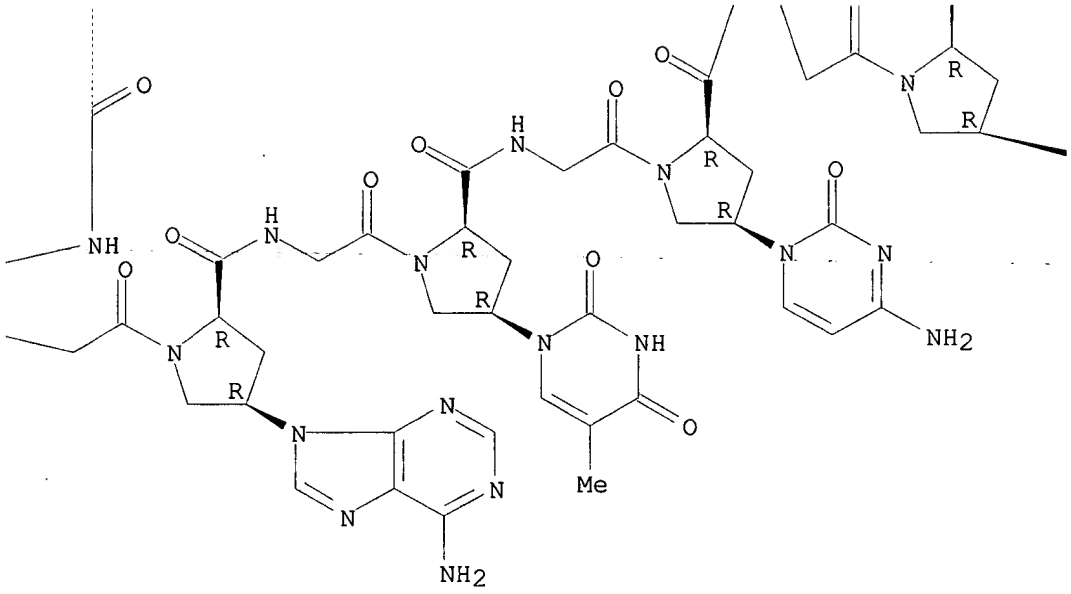

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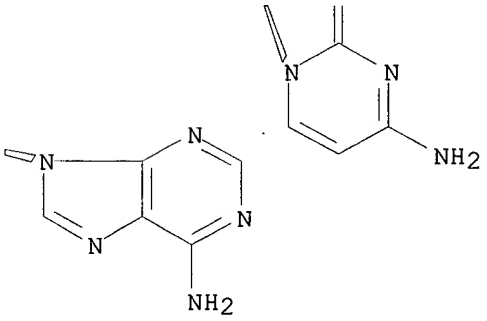


=> d ibib abs hitstr 9

L29 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:66698 HCAPLUS
DOCUMENT NUMBER: 128:241078
TITLE: **Polyamide** nucleic acid-DNA chimera lacking the **phosphate backbone** are novel primers for polymerase reaction catalyzed by DNA polymerases
AUTHOR(S): Misra, Hari S.; Pandey, Pradeep K.; Modak, Mukund J.; Vinayak, Ravi; Pandey, Virendra N.
CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, UMD-New Jersey Medical School, Newark, NJ, 07103, USA
SOURCE: Biochemistry (1998), 37(7), 1917-1925
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A peptide nucleic acid (PNA) oligomer, an analog of DNA, was examd. for its ability to function as a primer or a template to support DNA synthesis catalyzed by DNA polymerases. The analog, (PNA)19-TpG-OH, comprised of 19 bases in the form of PNA followed by a dinucleotide (TpG-OH) with a single **phosphate** and a free 3'OH terminus, was recognized as a bona fide primer by 2 reverse transcriptases and also by the Klenow fragment of E. coli DNA polymerase I. The 21-mer PNA chimera is extended on both RNA and DNA templates by all three polymerases. The specificity of binding of the PNA chimeric primer/DNA template at the template-primer binding site of the enzyme was shown by its photo-crosslinking ability to the enzyme which could be effectively competed out by another TP but not by template or primer alone. Furthermore, the chimeric TP-enzyme covalent complex was found to be catalytically active as judged by its ability to incorporate one nucleotide onto the 3'OH terminus of the immobilized primer. PNA sequences were also recognized as template when annealed with a DNA primer. These observations are in variance with the conventional suggestion that the **phosphate backbone** in the duplex region is essential for recognition and binding by DNA polymerases. The efficient extension of (PNA)19-TpG-OH suggests that the diam. of the duplex region of template primer rather than the **phosphate backbone** may be sufficient for recognition by DNA polymerases.

=> d ibib abs hitstr 10

L29 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:125535 HCAPLUS
DOCUMENT NUMBER: 122:2767
TITLE: Bridged, multiply-stranded oligonucleotides modified with non-nucleotide bridging groups
INVENTOR(S): Cook, Alan F.; Cohen, Jack S.; Gao, Hetian
PATENT ASSIGNEE(S): Pharmagenics, Inc., USA
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9415620	A1	19940721	WO 1994-US585	19940113
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2153057	AA	19940721	CA 1994-2153057	19940113

PRIORITY APPLN. INFO.: US 1993-4284 19930114

AB Double or triple stranded oligonucleotides in which the strands are connected by two bridging moieties (of which only one may be an oligonucleotide) that are bound to the **phosphate** moieties of the sugar **phosphate backbone** are described. Such oligonucleotides are designed to have increased resistance to exonucleases and endonucleases, greater thermal stabilities, improved cellular uptake, and improved binding to target proteins and nucleic acids. An oligonucleotide with two hexaethylene glycol bridging groups was synthesized by std. cyanoethyl phosphoramidite chem. using 4,4'-dimethoxytrityloxy-hexaethyleneoxy-2-cyanoethoxy-N,N'-diisopropylaminophosphine. The incorporation of dodecanediol, biotinylated dodecanediol, peptides, polyamines, polyalkylene thioglycols, substituted aroms., carbohydrates, and oligonucleotides is discussed or demonstrated. The Tms of triethylene glycol phosphodiester-bridged oligonucleotides was higher than that of a control oligonucleotide with a thymine pentamer of the same size. Hexaethylene glycol-bridged oligonucleotides were shown be much more resistant to mung bean nuclease and exonuclease III with half-lives increased >20-fold over control sequences. Bridged oligonucleotide analogs of the p53 tumor suppressor binding site bound to the protein although with lower efficiency than the unmodified sequences.

=> D IND 10

L29 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2002 ACS
IC ICM A61K031-70
ICS A61K031-74; A61K031-765; A61K031-785; A61K031-795; A61K048-00
CC 3-1 (Biochemical Genetics)
Section cross-reference(s): 1
ST oligonucleotide bridged synthesis
IT Polyamines
RL: MSC (Miscellaneous)
(as bridging group in bridged oligonucleotides)
IT Aromatic hydrocarbons, properties
RL: PRP (Properties)

(as bridging group in bridged oligonucleotides)
IT Peptides, properties
RL: PRP (Properties)
(as bridging group in bridged oligonucleotides)
IT **Polyamides**, properties
RL: PRP (Properties)
(as bridging group in bridged oligonucleotides)
IT Oligosaccharides
RL: MSC (Miscellaneous)
(in bridging group in bridged oligonucleotides)
IT Carbohydrates and Sugars, properties
RL: PRP (Properties)
(in bridging group in bridged oligonucleotides)
IT Hydrocarbons, properties
RL: PRP (Properties)
(sulfur-contg.; as bridging group in bridged oligonucleotides)
IT Thiols, properties
RL: PRP (Properties)
(di-, poly-, as bridging group in bridged oligonucleotides)
IT Molecular association
(intercalation, agents, in bridging group in bridged oligonucleotides)
IT Nucleotides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(oligo-, bridges, linear or circular; prepn. of, increased stability and resistance to nuclease digestion of)
IT Aromatic hydrocarbons, properties
RL: PRP (Properties)
(polycyclic, as bridging group in bridged oligonucleotides)
IT Alkenes, biological studies
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(polymers, as bridging group in bridged oligonucleotides)
IT 9026-81-7, Nuclease 9055-11-2, Endonuclease 37228-74-3, Exonuclease
RL: USES (Uses)
(bridged oligonucleotides with increased resistance to)
IT 158665-27-1P 158665-28-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reactions of, in prepn. bridged oligonucleotides)
IT 159608-73-8P 159608-74-9P 159608-75-0P
RL: PREP (Preparation)
(prepn. of, binding to p53 protein of, effects of alkylene glycol bridging moieties on binding of)
IT 159577-14-7P 159608-67-0P 159608-68-1P 159608-69-2P 159608-70-5P
RL: PREP (Preparation)
(prepn. of, bridged oligonucleotides for diagnostics and therapeutics in relation to)
IT 159410-44-3P 159410-45-4P 159410-46-5P 159410-47-6P 159608-71-6P
159608-72-7P
RL: PREP (Preparation)
(prepn. of, thermostability of, effects of alkylene glycol bridging moieties on thermal stability in relation to)
IT 39529-98-1, Dodecanediol 40615-36-9, Dimethoxytrityl chloride
89992-70-1
RL: RCT (Reactant)
(reactions of, in prepn. dimethoxytrityldodecanediol cyanoethoxy diisopropylaminophosphine for prepn. dodecanediol-bridged oligonucleotides)
IT 125607-09-2
RL: RCT (Reactant)
(reactions of, in prepn. hexaethylene glycol bridged oligonucleotides)

=> d ibib abs hitstr 11

L29 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:625316 HCAPLUS
DOCUMENT NUMBER: 121:225316
TITLE: Analyzing DNA complexes by circular and linear dichroism
AUTHOR(S): Norden, Bengt; Kurucsev, Tomas
CORPORATE SOURCE: Dep. Physical Chem., Chalmers Univ. Technology, Goeteborg, S-142 96, Swed.
SOURCE: J. Mol. Recognit. (1994), 7(2), 141-55
CODEN: JMORE4; ISSN: 0952-3499
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with many refs. Application of linear dichroism (LD) and CD in nucleic acid research is illustrated by recent results aimed at answering specific structural problems in the interaction of DNA with mols. of biol. importance. The authors first consider the circumstances under which ligands, such as DAPI (4',6-diamidino-2-phenylindole), change their preferred binding mode in the minor groove to major groove binding or intercalation. As an extension of this problem the authors refer to the switch between groove binding and intercalation of structurally similar ligands such as ellipticines and trigonal ruthenium complexes. They also explore the use of LD and CD in detn. of the structure of the complex formed between the polynucleotide poly(dA) and the novel 'peptide nucleic acid', consisting of nucleic acid bases joined by a **polyamide** homomorphous with the deoxyribose-**phosphate backbone** of DNA. Finally, the structure and interaction of the recombination enzyme RecA with DNA is discussed, in particular the influence of the presence of intercalators, groove binders or covalent DNA adducts.

=> d ibib abs hitstr 12

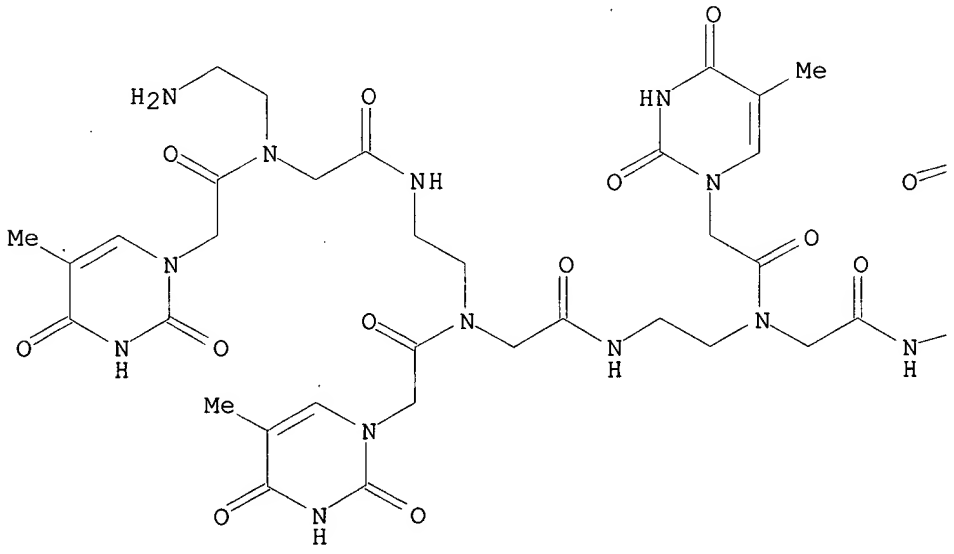
L29 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1992:146300 HCAPLUS
DOCUMENT NUMBER: 116:146300
TITLE: Sequence-selective recognition of DNA by strand displacement with a thymine-substituted **polyamide**
AUTHOR(S): Nielsen, Peter E.; Egholm, Michael; Berg, Rolf H.; Buchardt, Ole
CORPORATE SOURCE: Res. Cent. Biotechnol., Panum Inst., Copenhagen, DK-2200 N, Den.
SOURCE: Science (Washington, D. C., 1883-) (1991), 254(5037), 1497-500
CODEN: SCIEAS; ISSN: 0036-8075
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A **polyamide** nucleic acid (PNA) was designed by detaching the deoxyribose **phosphate backbone** of DNA in a computer model and replacing it with an achiral **polyamide** backbone. On the basis of this model, oligomers consisting of thymine-linked aminoethylglycyl units were prepd. These oligomers recognize their complementary target in double-stranded DNA by strand displacement. The displacement is made possible by the extraordinarily high stability of the PNA-DNA hybrids. The results show that the backbone of DNA can be replaced by a **polyamide**, with the resulting oligomer retaining base-specific hybridization.

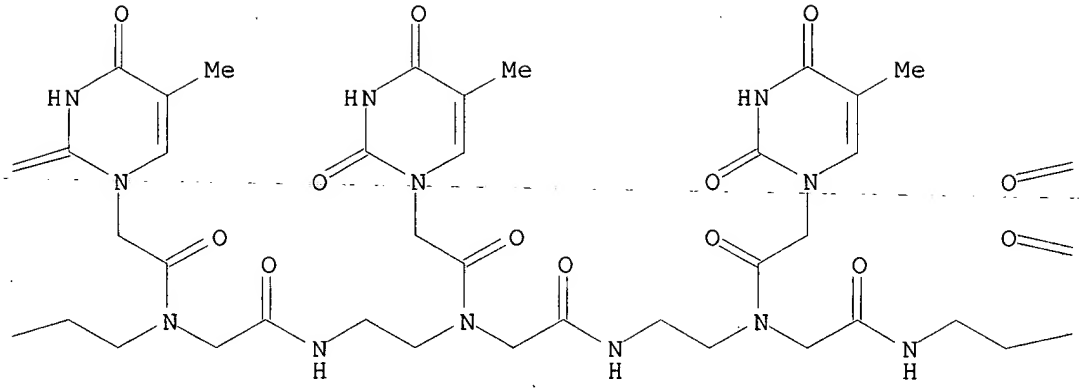
IT **139574-70-2P 139628-82-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and DNA sequence-selective recognition by)
RN 139574-70-2 HCAPLUS
CN Peptide nucleic acid, (H-T-T-T-T-T-T-T-T-T-T)-Lys-NH2, conjugate monoacid (9CI) (CA INDEX NAME)

Absolute stereochemistry.

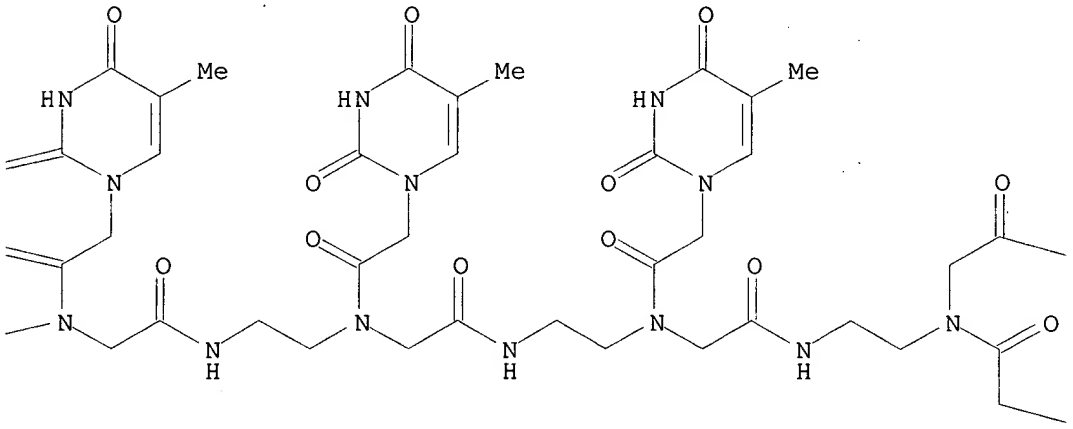
PAGE 1-A



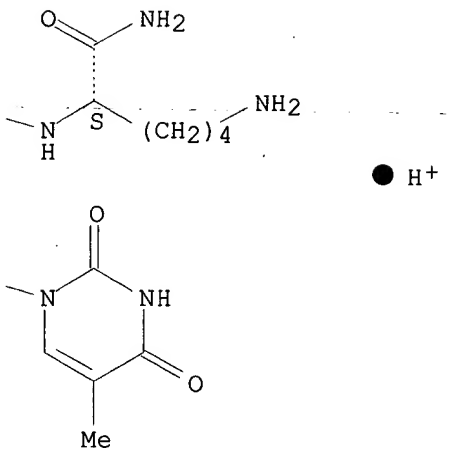
PAGE 1-B



PAGE 1-C



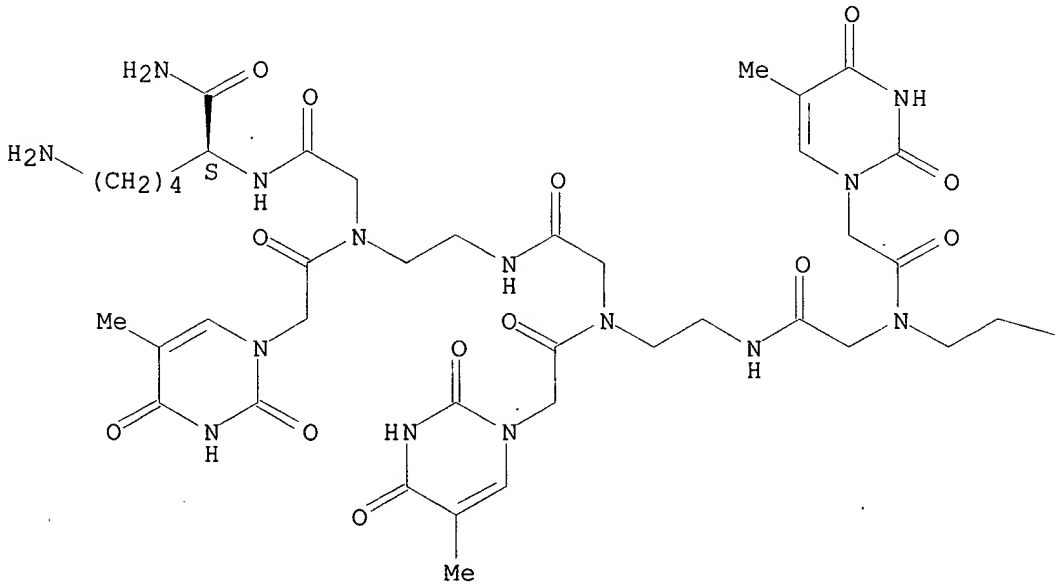
PAGE 1-D



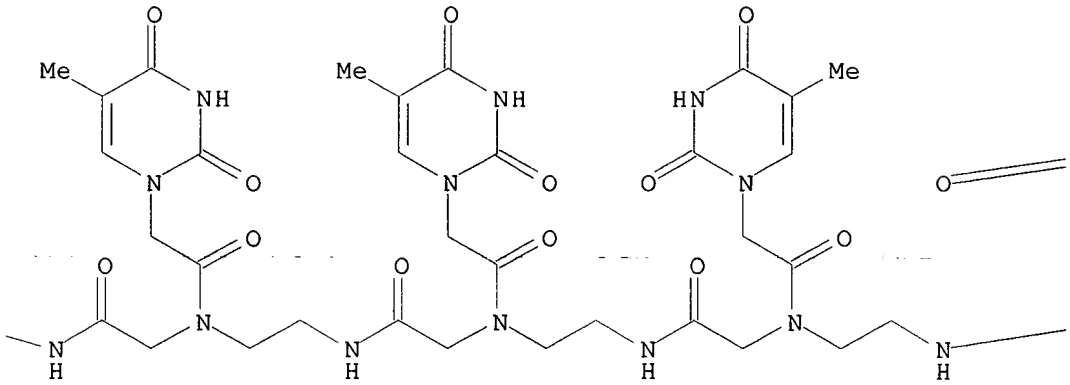
RN 139628-82-3 HCAPLUS
CN Peptide nucleic acid, ([6-[[[9-[[6-[(4-nitrobenzoyl)amino]hexyl]amino]-4-acridinyl]carbonyl]amino]-1-oxohexyl]-T-T-T-T-T-T-T-T-T-T)-Lys-NH2, conjugate diacid (9CI) (CA INDEX NAME)

Absolute stereochemistry.

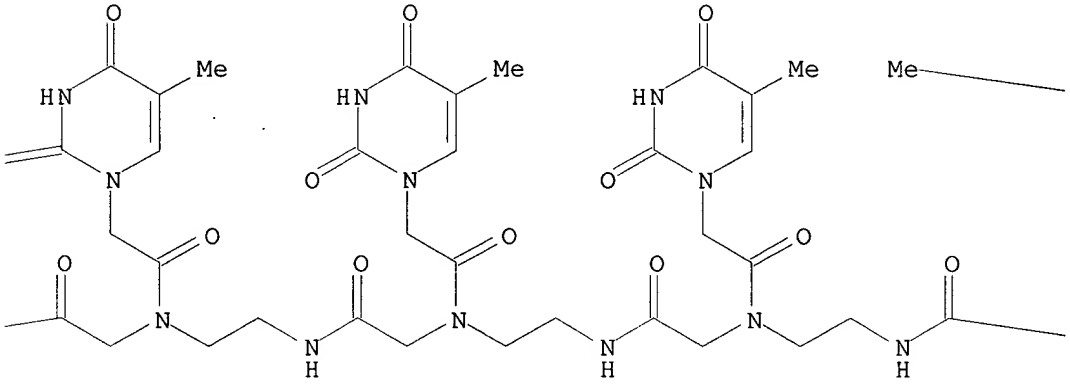
PAGE 1-A



PAGE 1-B



PAGE 1-C



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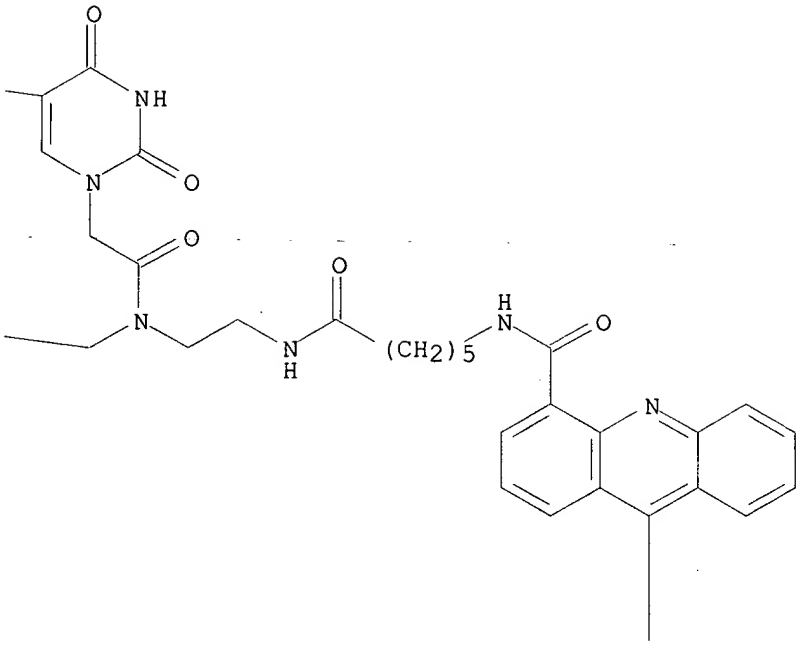
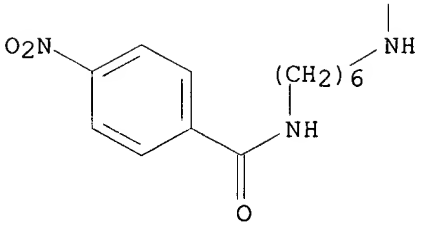


PAGE 2-A

●2 H^+

PAGE 2-D



=> d ibib abs hitstr 13

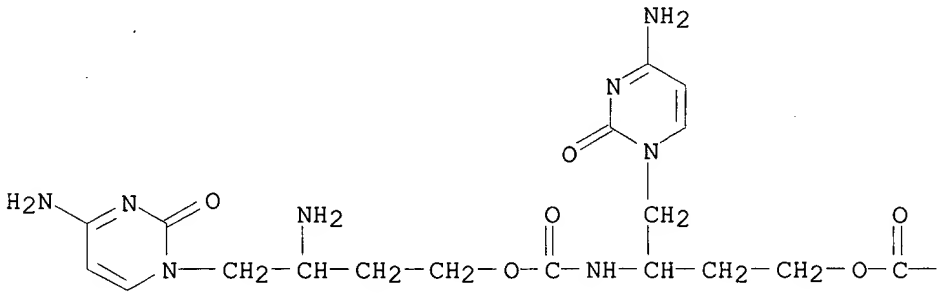
L29 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:578713 HCAPLUS
DOCUMENT NUMBER: 115:178713
TITLE: Molecular modeling of acyclic **polyamide** oligonucleotide analogs
AUTHOR(S): Weller, Dwight D.; Daly, Daniel T.; Olson, Wilma K.; Summerton, James E.
CORPORATE SOURCE: Dep. Chem., Oregon State Univ., Corvallis, OR, 97331-4003, USA
SOURCE: J. Org. Chem. (1991), 56(21), 6000-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The feasibility of replacing the sugar-**phosphate backbone** of nucleic acids with a **polyamide**-type backbone was investigated by using mol. modeling techniques that exam. the ability of the acyclic backbone to adopt low energy conformations that conform to the nucleic acid A- and B-form helixes. Of the several backbone possibilities examd. (nylons, polyurethanes, polypeptides), the most favorable appear to be those derived from a polypeptide. For most of the cases studied, the models predict a preference for binding of a given backbone type to either A- or B-form targets and, in some cases, suggest an orientational bias for direction along the helical axis, or a preferred stereochem. at stereogenic atoms in the backbone.

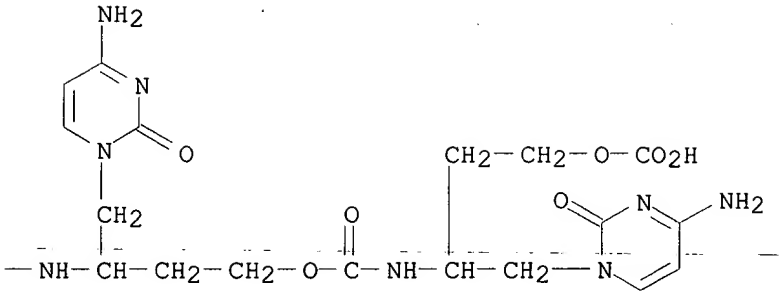
IT **136277-55-9 136277-56-0 136301-88-7**
136301-89-8 136301-90-1 136376-53-9
RL: PRP (Properties)
(energy of, mol. modeling in relation to)

RN 136277-55-9 HCAPLUS
CN 2,8,14-Trioxa-6,12,18-triazanonadecanedioic acid, 5,11,17-tris[(4-amino-2-oxo-1(2H)-pyrimidinyl)methyl]-7,13-dioxo-, 19-[3-amino-4-(4-amino-2-oxo-1(2H)-pyrimidinyl)butyl] ester, [5R-[5R*,11R*,17R*,19(R*)]]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



RN 136277-56-0 HCAPLUS
CN Glycine, N-[3-(4-amino-2-oxo-1(2H)-pyrimidinyl)-N-[N-[3-(4-amino-2-oxo-1(2H)-pyrimidinyl)-N-[N-[3-(4-amino-2-oxo-1(2H)-pyrimidinyl)-N-[N-[3-(4-amino-2-oxo-1(2H)-pyrimidinyl)-D-alanyl]glycyl]-D-alanyl]glycyl]-D-alanyl]glycyl]-D-alanyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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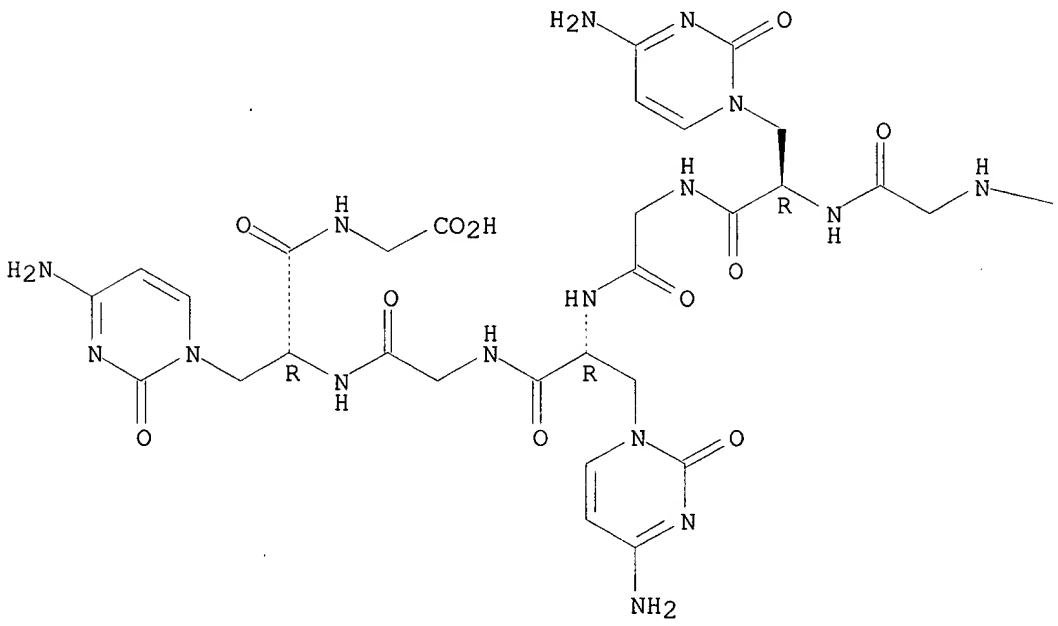

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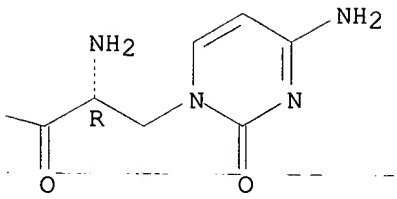

RN 136301-88-7 HCAPLUS
CN 1(2H)-Pyrimidinebutanoic acid, 4-amino-.gamma.-[[[5-[[5-[[5-amino-4-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxopentyl]amino]-4-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxopentyl]amino]-4-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxopentyl]amino]methyl]-2-oxo-, [.gamma.S-[.gamma.R*[R*[R*(R*)]]]]- (9CI) (CA INDEX NAME)

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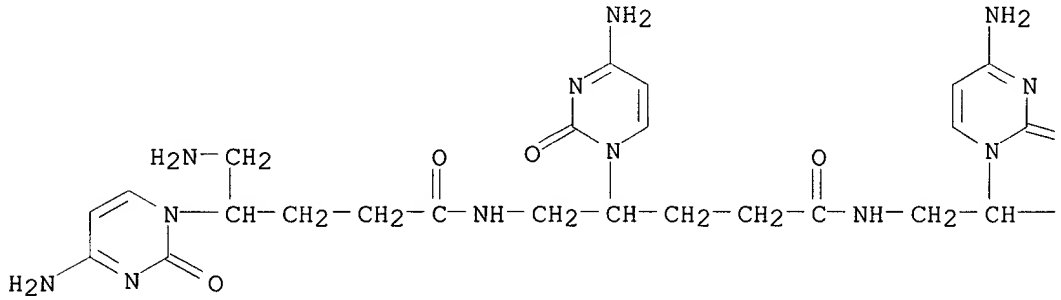

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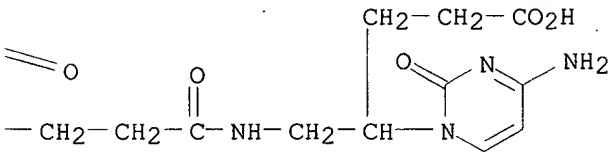

RN 136301-89-8 HCAPLUS
CN 1(2H)-Pyrimidinepentanoic acid, 4-amino-.gamma.-[[4-[[4-[[4-amino-5-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxopentyl]amino]-5-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxopentyl]amino]-5-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxopentyl]amino]-2-oxo-, [.gamma.R-[.gamma.R*[R*[R*(R*)]]]]- (9CI) (CA INDEX NAME)

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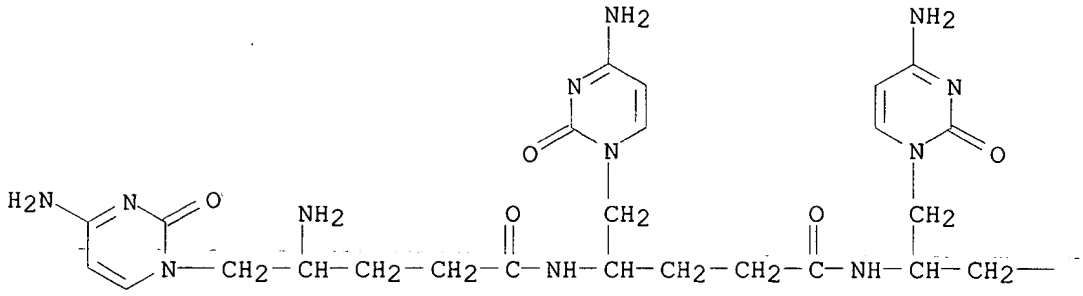

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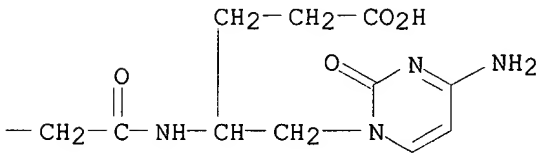
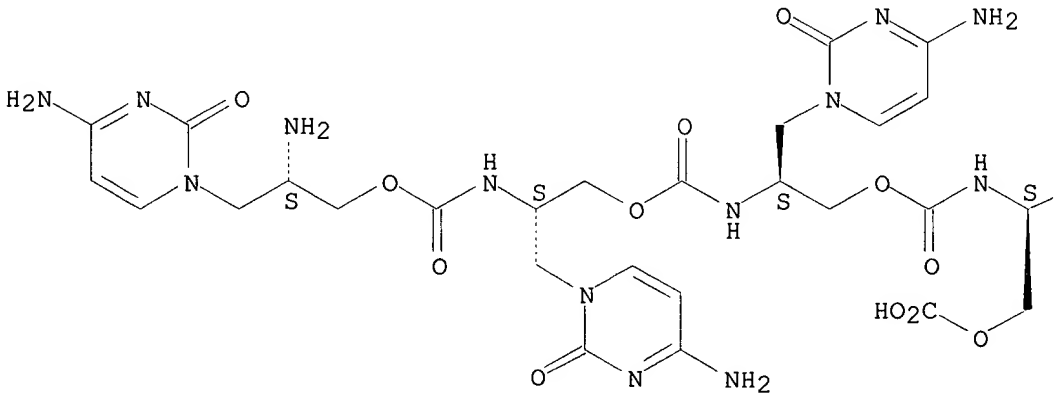


RN 136301-90-1 HCAPLUS
CN 2,7,12-Trioxa-5,10,15-triazahexadecanedioic acid, 4,9,14-tris[(4-amino-2-oxo-1(2H)-pyrimidinyl)methyl]-6,11-dioxo-, 16-[2-amino-3-(4-amino-2-oxo-1(2H)-pyrimidinyl)propyl] ester, [4S-[4R*,9R*,14R*,16(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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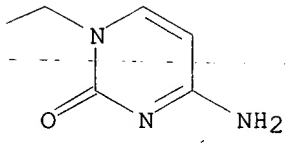

RN 136376-53-9 HCAPLUS
CN 1(2H)-Pyrimidinehexanoic acid, 4-amino-.delta.-[[5-[[5-[[5-amino-6-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxohexyl]amino]-6-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxohexyl]amino]-6-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxohexyl]amino]-2-oxo-, [.delta.S-[.delta.R*[R*[R*(R*)]]]]- (9CI) (CA INDEX NAME)

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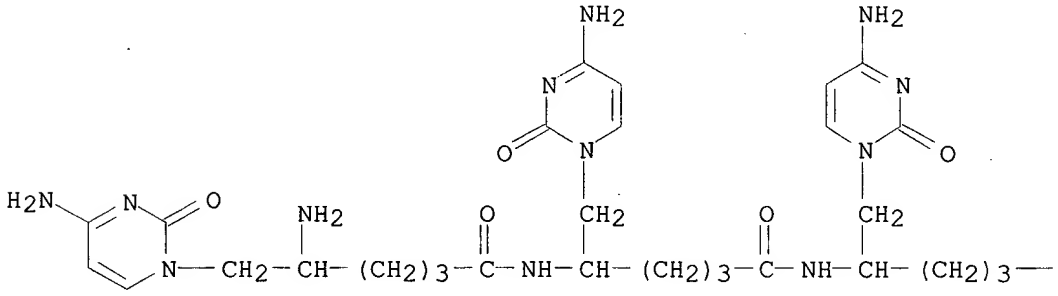

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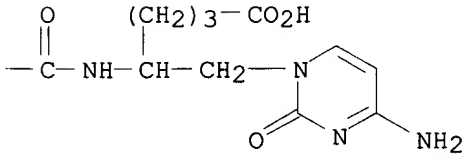
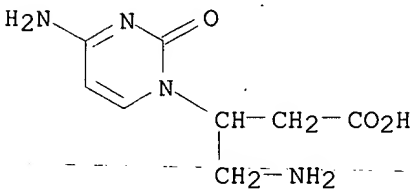


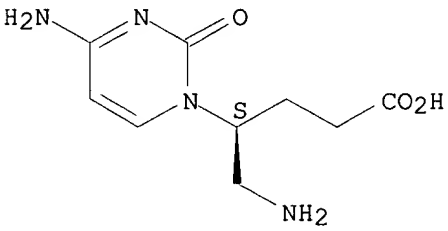
IT **136277-48-0 136277-49-1 136277-50-4**
136277-51-5 136277-52-6 136277-53-7
136277-54-8 136301-87-6
RL: ANST (Analytical study)
(mol. modeling of, nucleic acid binding in relation to)

RN 136277-48-0 HCAPLUS
CN 1(2H)-Pyrimidinepropanoic acid, 4-amino-.beta.-(aminomethyl)-2-oxo- (9CI) (CA INDEX NAME)

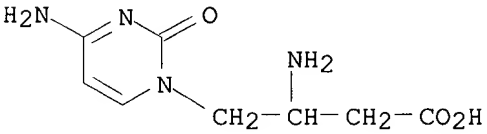


RN 136277-49-1 HCAPLUS
CN 1(2H)-Pyrimidinebutanoic acid, 4-amino-.gamma.-(aminomethyl)-2-oxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

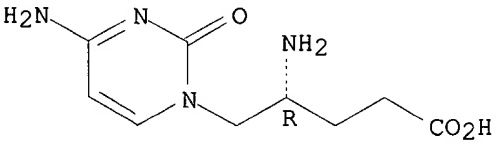


RN 136277-50-4 HCAPLUS
CN 1(2H)-Pyrimidinebutanoic acid, .beta.,4-diamino-2-oxo- (9CI) (CA INDEX NAME)



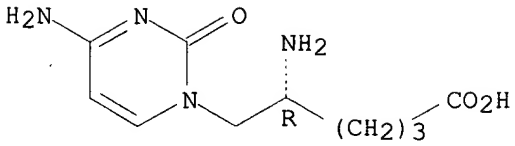
RN 136277-51-5 HCAPLUS
CN 1(2H)-Pyrimidinepentanoic acid, .gamma.,4-diamino-2-oxo-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



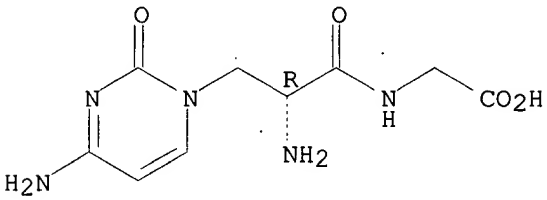
RN 136277-52-6 HCAPLUS
CN 1(2H)-Pyrimidinehexanoic acid, .delta.,4-diamino-2-oxo-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



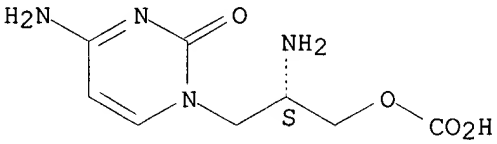
RN 136277-53-7 HCAPLUS
CN Glycine, N-[3-(4-amino-2-oxo-1(2H)-pyrimidinyl)-D-alanyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



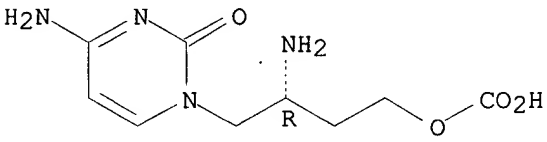
RN 136277-54-8 HCAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-[2-amino-3-(carboxyoxy)propyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



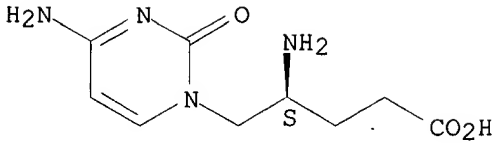
RN 136301-87-6 HCAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-[2-amino-4-(carboxyoxy)butyl]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



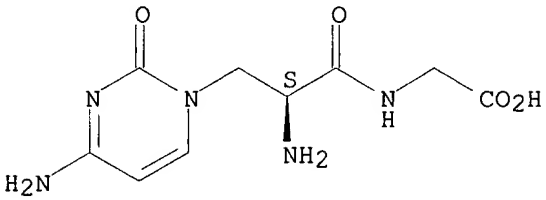
IT **136277-57-1P 136277-58-2P 136277-59-3P**
136277-60-6P 136277-61-7P 136277-62-8P
136327-73-6P 136375-16-1P 136376-54-0P
RL: PREP (Preparation)
(prepn. of)
RN 136277-57-1 HCAPLUS
CN 1(2H)-Pyrimidinepentanoic acid, .gamma.,4-diamino-2-oxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 136277-58-2 HCAPLUS
CN Glycine, N-[3-(4-amino-2-oxo-1(2H)-pyrimidinyl)-L-alanyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 136277-59-3 HCAPLUS
CN 1(2H)-Pyrimidinehexanoic acid, 4-amino-.delta.-[[5-[[5-[[5-amino-6-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxohexyl]amino]-6-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxohexyl]amino]-6-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxohexyl]amino]-2-oxo-, [.delta.R-[.delta.R*[R*[R*(R*)]]]]- (9CI) (CA INDEX NAME)

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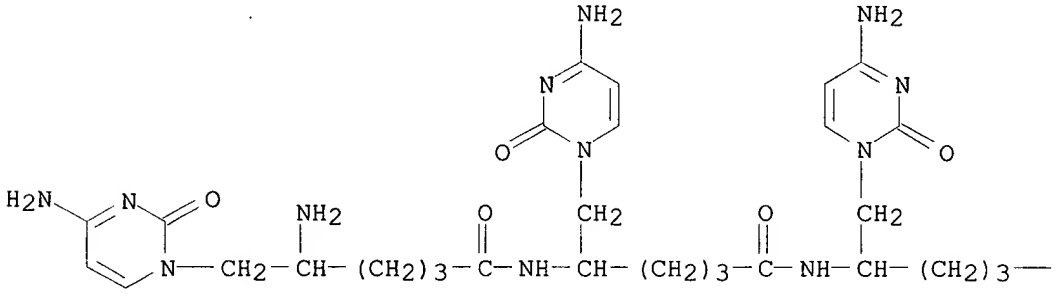

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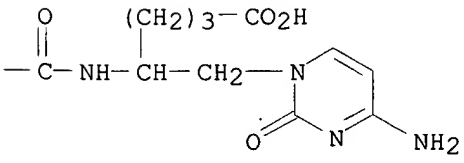
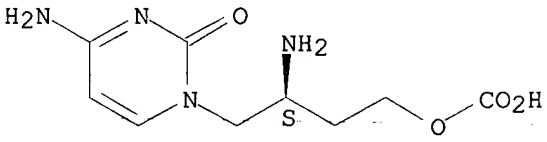


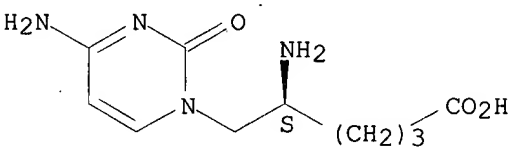
RN 136277-60-6 HCAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-[2-amino-4-(carboxyoxy)butyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 136277-61-7 HCAPLUS
CN 1(2H)-Pyrimidinehexanoic acid, .delta.,4-diamino-2-oxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 136277-62-8 HCAPLUS
CN Glycine, 3-(4-amino-2-oxo-1(2H)-pyrimidinyl)alanylglycyl-3-(4-amino-2-oxo-1(2H)-pyrimidinyl)alanylglycyl-3-(4-amino-2-oxo-1(2H)-pyrimidinyl)alanylglycyl-3-(4-amino-2-oxo-1(2H)-pyrimidinyl)alanyl- (9CI) (CA INDEX NAME)

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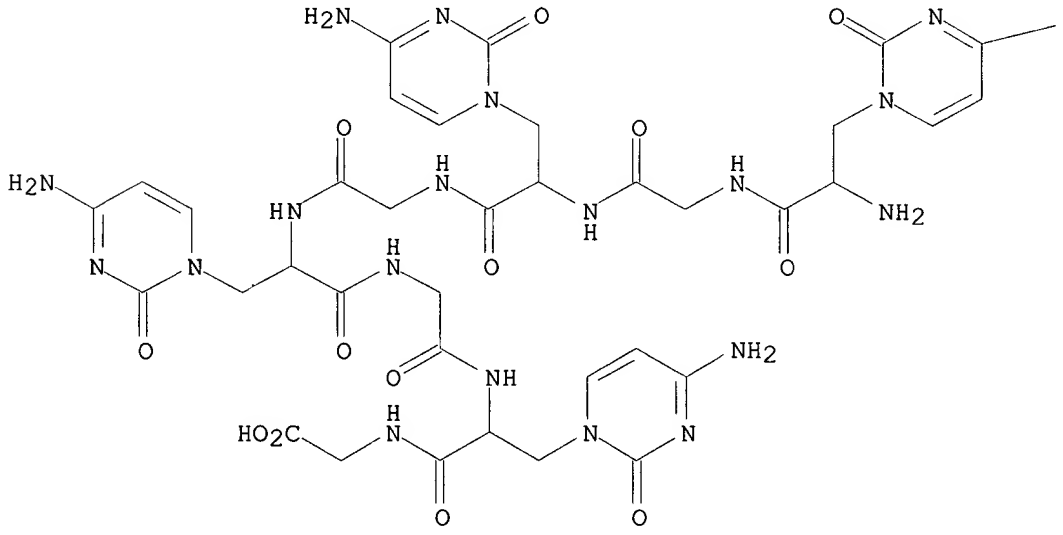

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—NH_2

RN 136327-73-6 HCAPLUS
CN Glycine, N-[3-(4-amino-2-oxo-1(2H)-pyrimidinyl)-N-[N-[3-(4-amino-2-oxo-1(2H)-pyrimidinyl)-N-[N-[3-(4-amino-2-oxo-1(2H)-pyrimidinyl)-N-[N-[3-(4-amino-2-oxo-1(2H)-pyrimidinyl)-L-alanyl]glycyl]-L-alanyl]glycyl]-L-alanyl]glycyl]-L-alanyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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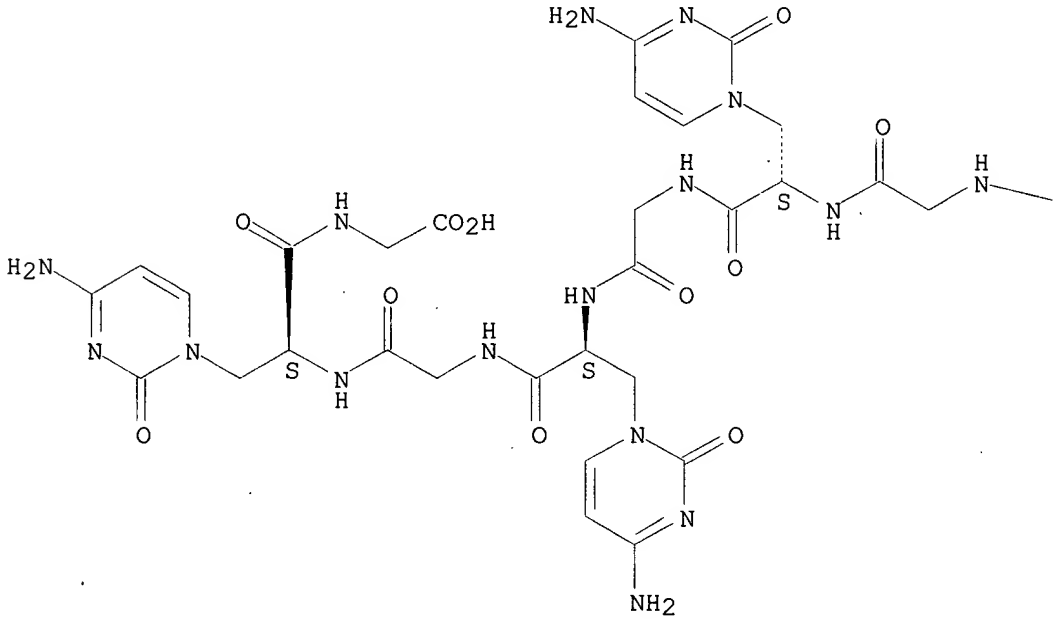

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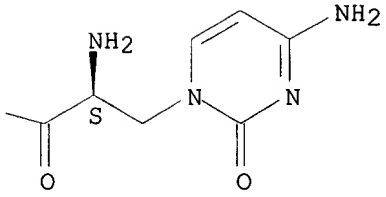

RN 136375-16-1 HCAPLUS
CN 2,8,14-Trioxa-6,12,18-triazanonadecanedioic acid, 5,11,17-tris[(4-amino-2-oxo-1(2H)-pyrimidinyl)methyl]-7,13-dioxo-, 19-[3-amino-4-(4-amino-2-oxo-1(2H)-pyrimidinyl)butyl] ester, [5S-[5R*,11R*,17R*,19(R*)]]- (9CI) (CA

INDEX NAME)

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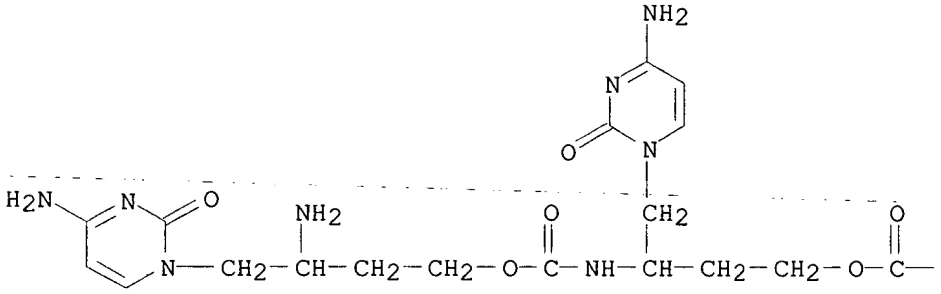

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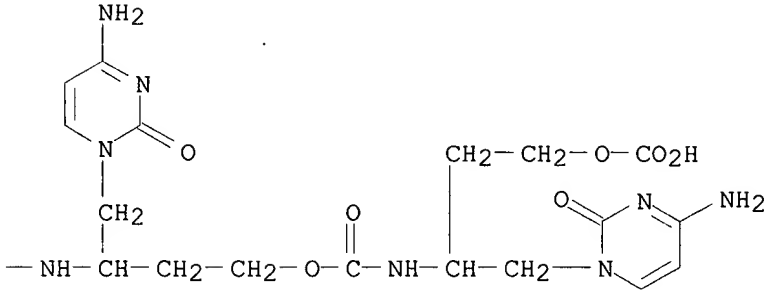

RN 136376-54-0 HCAPLUS
CN 1(2H)-Pyrimidinepentanoic acid, 4-amino-.gamma.-[[4-[[4-[[4-amino-5-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxopentyl]amino]-5-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxopentyl]amino]-5-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1-oxopentyl]amino]-2-oxo-, [.gamma.S-[.gamma.R*[R*[R*(R*)]]]]- (9CI) (CA INDEX NAME)

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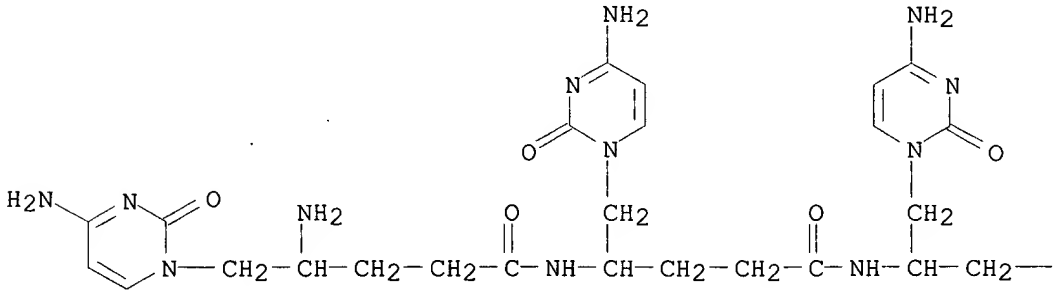

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